Clustering

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(some material taken or adapted from slides by Hinrich Schutze)

Clustering
objective

- Grouping documents or instances into subsets or clusters
- Documents within a the same cluster should be similar
- Documents from different clusters should be dissimilar
- A common form of unsupervised learning
- Unsupervised = no human-produced labels
- The goal is to discover structure from the data

Clustering vs. Classification

- Classification:
    - the input to the system is a set of labeled data
    - the algorithm learns a model for predicting the label on new examples
- Clustering:
    - the input the system is a set of unlabeled data
    - the algorithm infers the labels from the data and assigns a label to each input instance

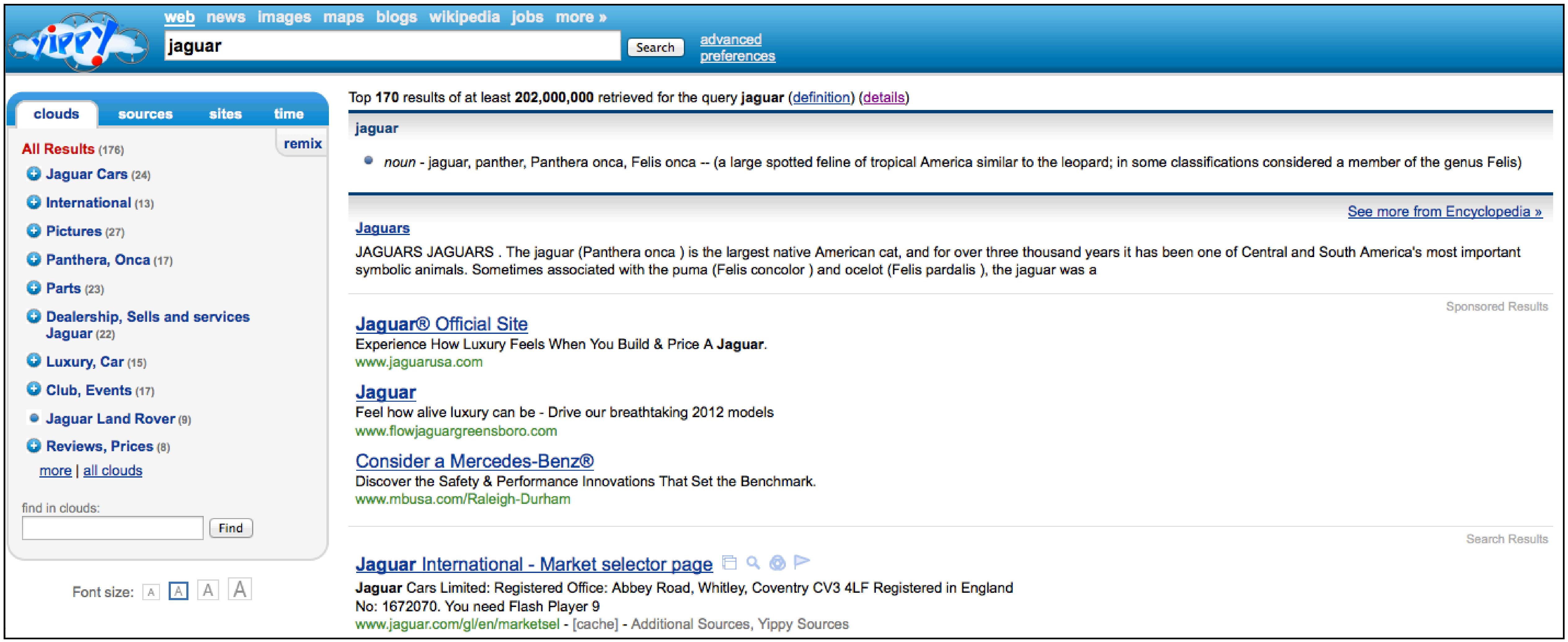
Clustering

applications

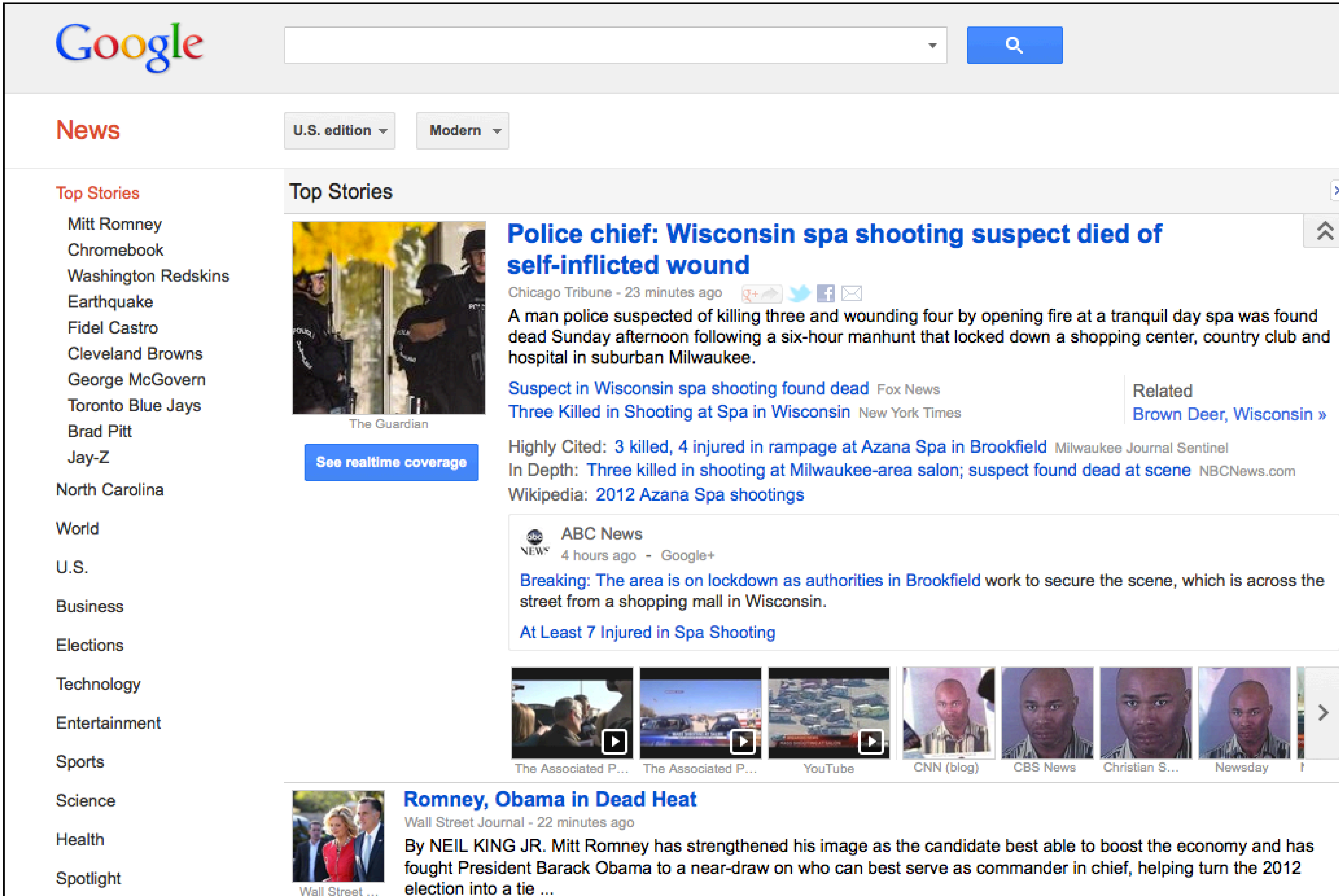
- Search engine results clustering: grouping search engine results by topic
  - the user can identify the relevant clusters and ignore the non-relevant ones
- Collection clustering: grouping documents by topic to support navigation and exploration
- Data analytics: grouping instances to identify popular trends (big clusters) and outliers (small clusters)

Clustering Applications

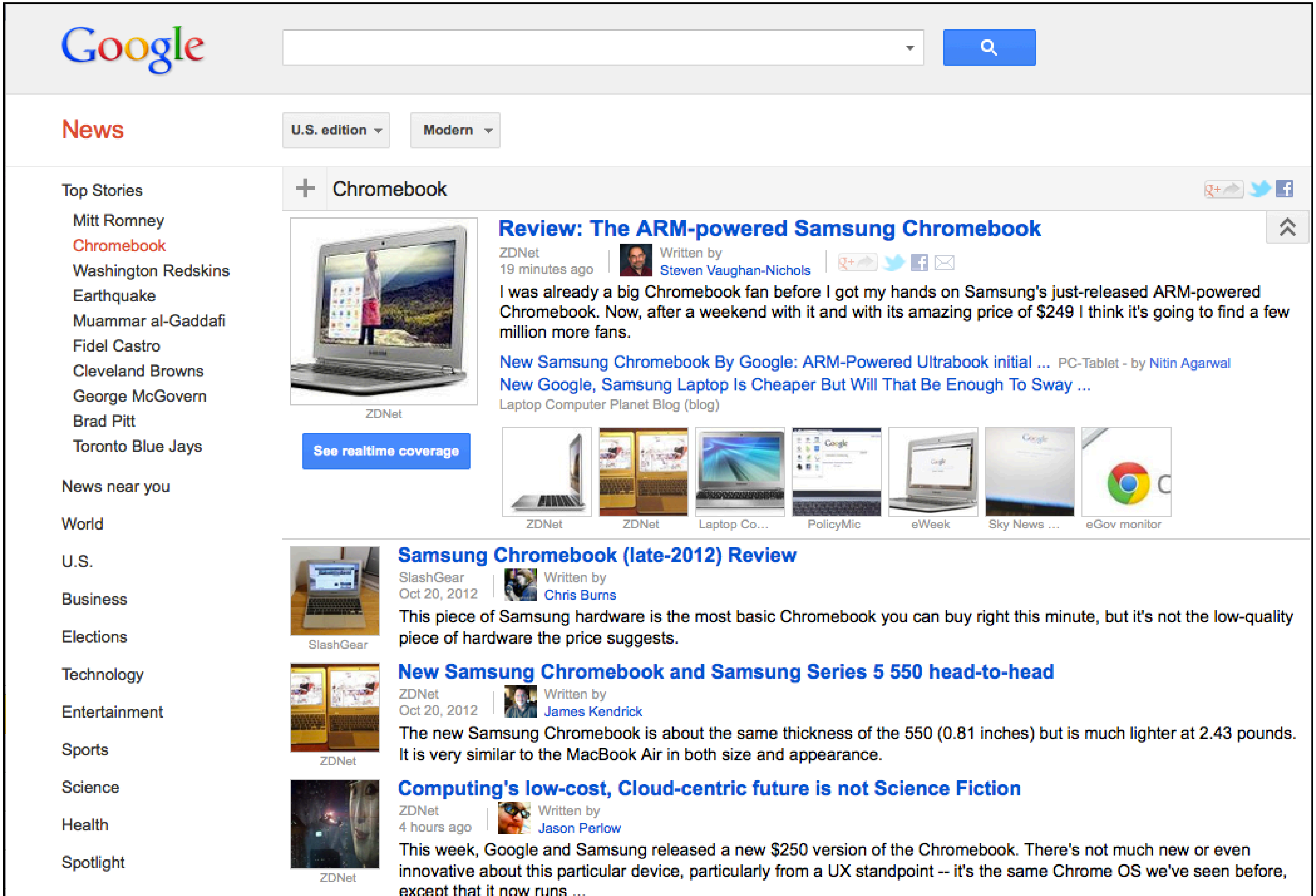
search engine results clustering



Clustering Applications
collection clustering



Clustering Applications
collection clustering



Clustering
objective

- Grouping documents or instances into subsets or clusters
- Documents within a the same cluster should be similar
- Documents from different clusters should be dissimilar

Clustering
basics

- What does it mean for documents to be "similar" or "dissimilar"?

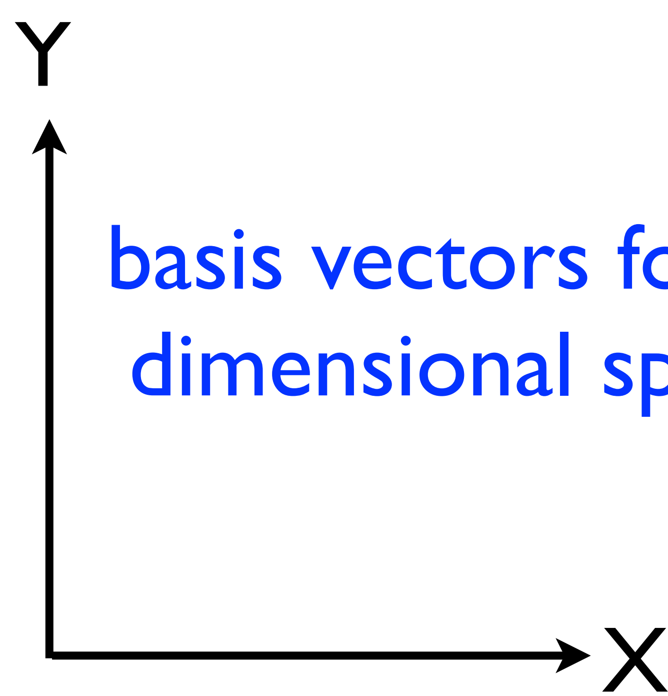
Clustering
basics

- What does it mean for documents to be similar or dissimilar?
- We need a computational way of modeling similarity
- One solution: model similarity using distance in a vector space representation of the collection or dataset
  - small distance = high similarity
  - long distance = low similarity

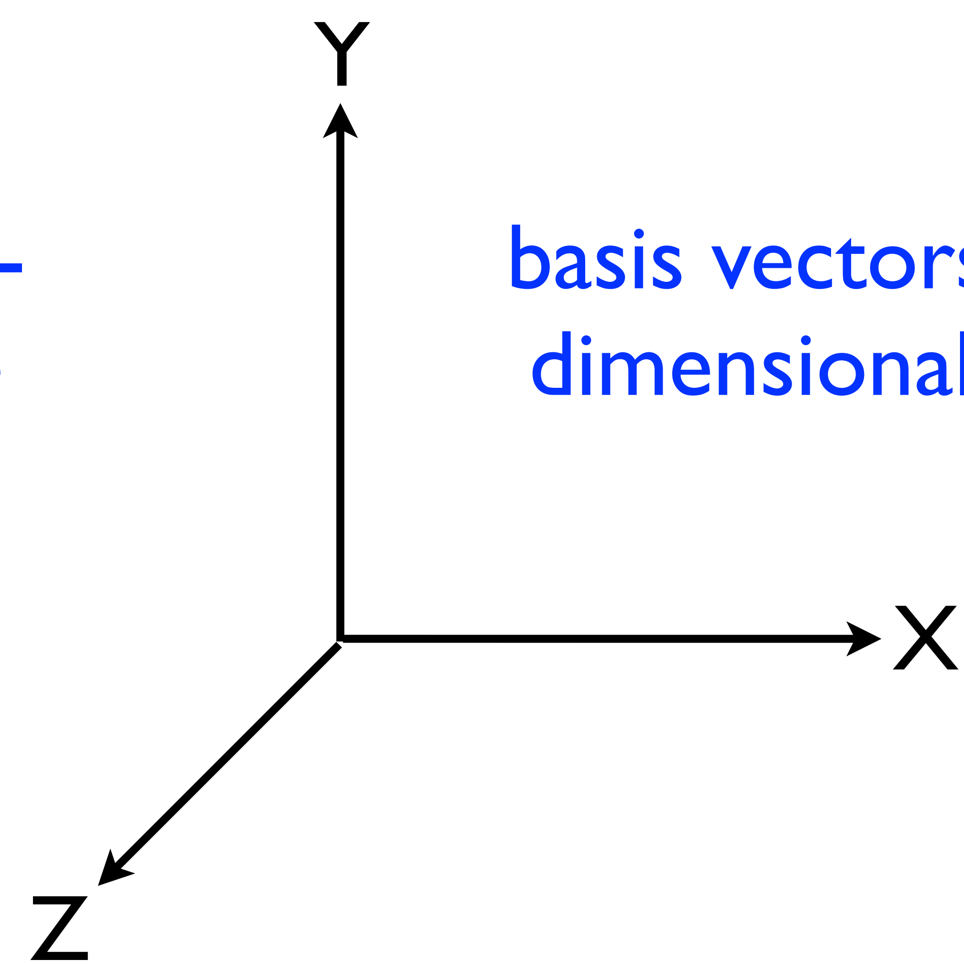
Vector Space Representation

review

- A vector space is defined by a set of linearly independent basis vectors
- The basis vectors correspond to the dimensions or directions of the vector space



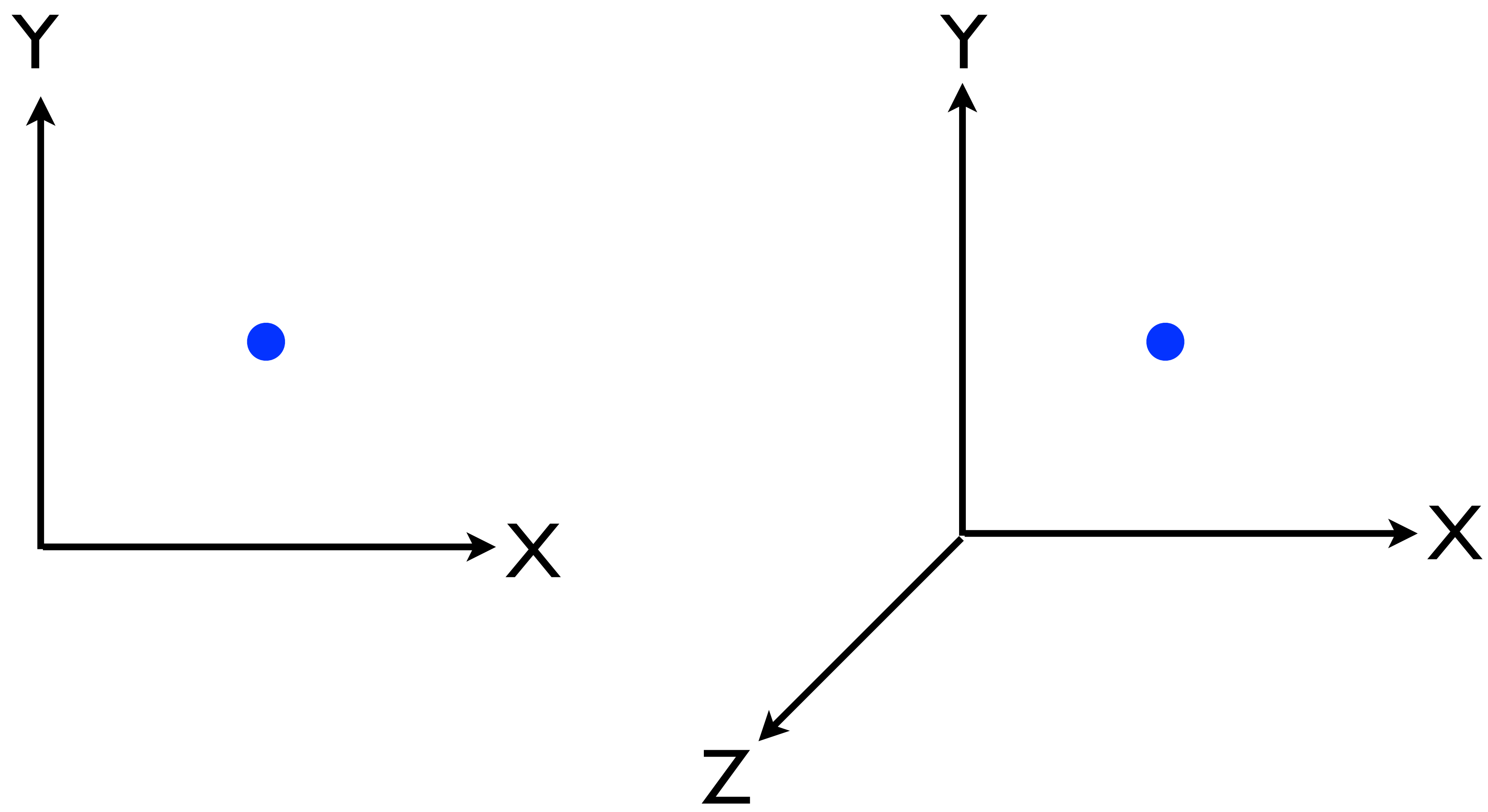
basis vectors for 2-dimensional space



basis vectors for 3-dimensional space

Vector Space Representation
review

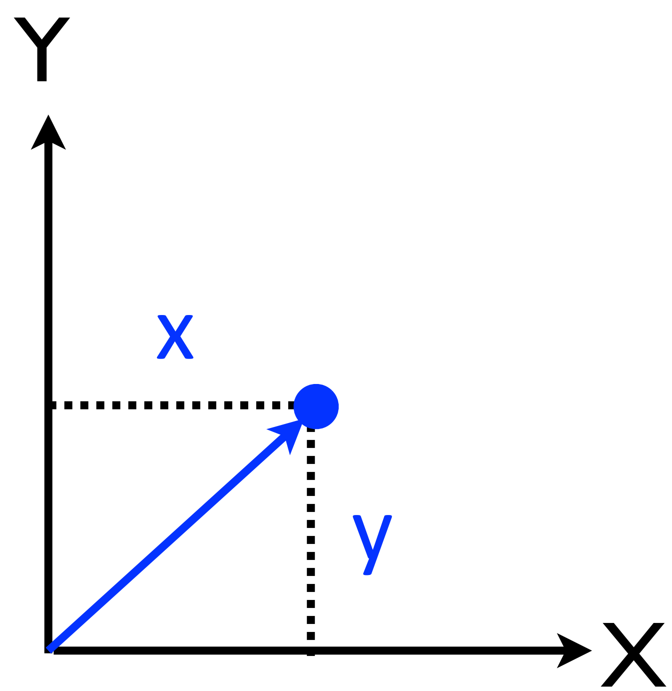
- A vector is a point in a vector space

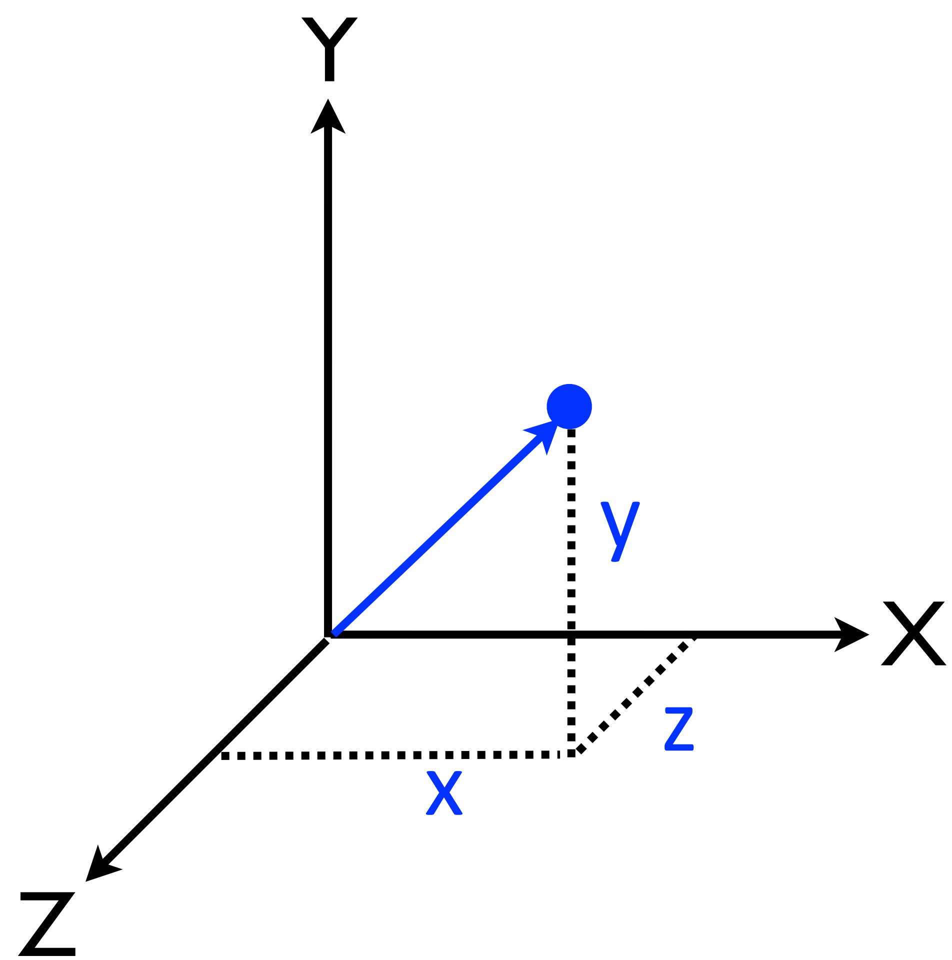


Vector Space Representation

review

- A 2-dimensional vector can be written as [x,y]
- A 3-dimensional vector can be written as [x,y,z]





Vector Space Representation

review

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
1	0	1	0	1	0	0	1	1	0
0	1	0	1	1	0	1	1	0	0
0	1	0	1	1	0	1	0	0	0
0	0	1	0	1	1	0	1	1	1
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
1	1	0	1	1	0	0	1	0	1

Vector Space Representation
review

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
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⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
1	1	0	1	1	0	0	1	0	1

- We can represent this document as a vector in a 10-dimensional vector space

Vector Space Representation

review

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
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0	1	0	1	1	0	1	1	0	0
0	1	0	1	1	0	1	0	0	0
0	0	1	0	1	1	0	1	1	1
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
1	1	0	1	1	0	0	1	0	1

- This representation assumes binary term-weights.
- Are there other term-weighting schemes?

TF, IDF, or TF.IDF?

adrain adrian all already also an and apartment apollo as aspiring at balboa become better big boxer boxing but by can career champion chance creed current debt doesn earns every exhibition extra far fight for gazzo gets girl go has he heavyweight her himself his if in is it keep later life living loan lovers make man match meat men mickey named nobody of paulie pet philadelphia rocky set she shot small somebody someone still store struggling supplies surprised that the they think this through time title to trainer training up want when where who willing with woman won works

TF, IDF, or TF.IDF?

ability adrain adrian already apartment apollo aspiring balboa become befriended befriends big boxer boxes boxing canvas champion chance checks chooses collecting collector creed current deadbeats debt debts distance doesn downtown earns ease easily exhibition extra extremely factory fight forgot gazzo gear gotten heavyweight his is jergens later loan lot lovers managers match meat mickey named nobody odds packing paulie pennsylvania pet philadelphia pittance promoter publicity ready rocky sells set shark sharp shot shy somebody someone stallion store struggling stunt supplies supposed surprised thanksgiving think thrilled time title touting trainer training triumph up ve viciousness visits where who willing won works

TF, IDF, or TF.IDF?

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mickey nobody odds packing paulie pennsylvania pet
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ready rocky sells shark sharp shop shy skills somebody spends
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Vector Space Representation

review

- Similarity = Euclidean Distance:

$$D(x,y) = \sqrt{\left(\sum_{i=1}^{|\mathcal{V}|}(x_i - y_i)^2\right)}$$

Vector Space Representation

review

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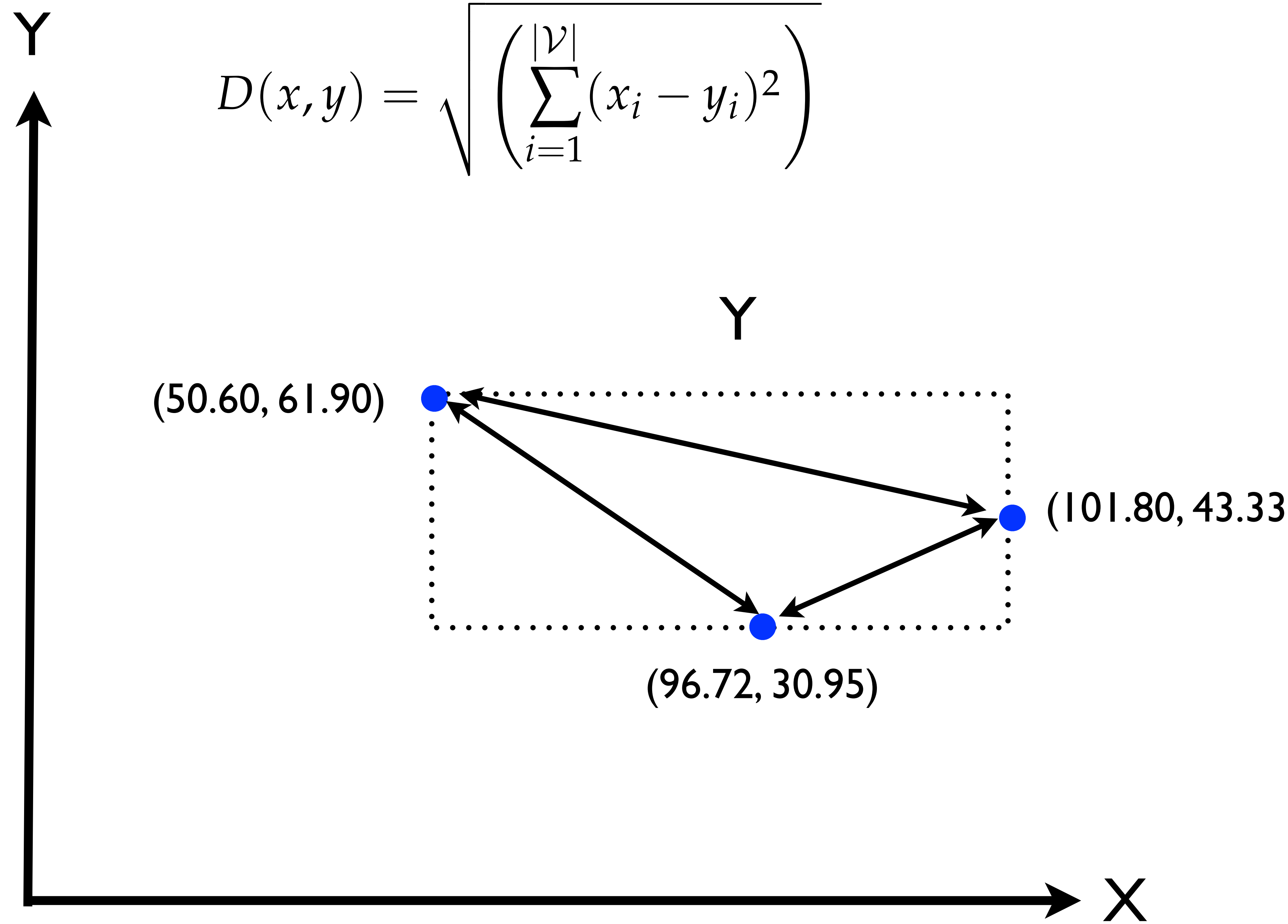
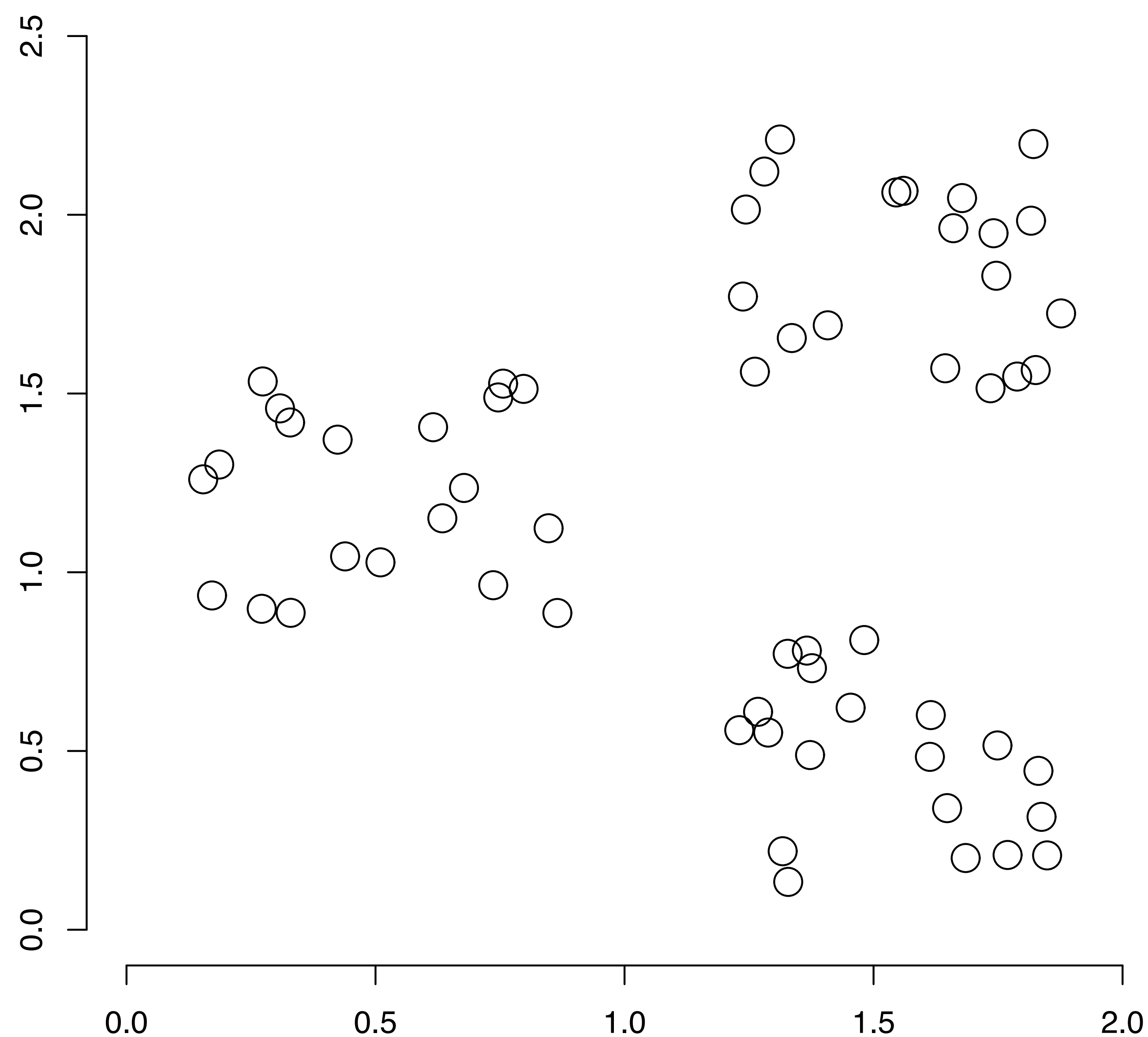


Clustering

- What would we expect a clustering algorithm to do with this dataset?



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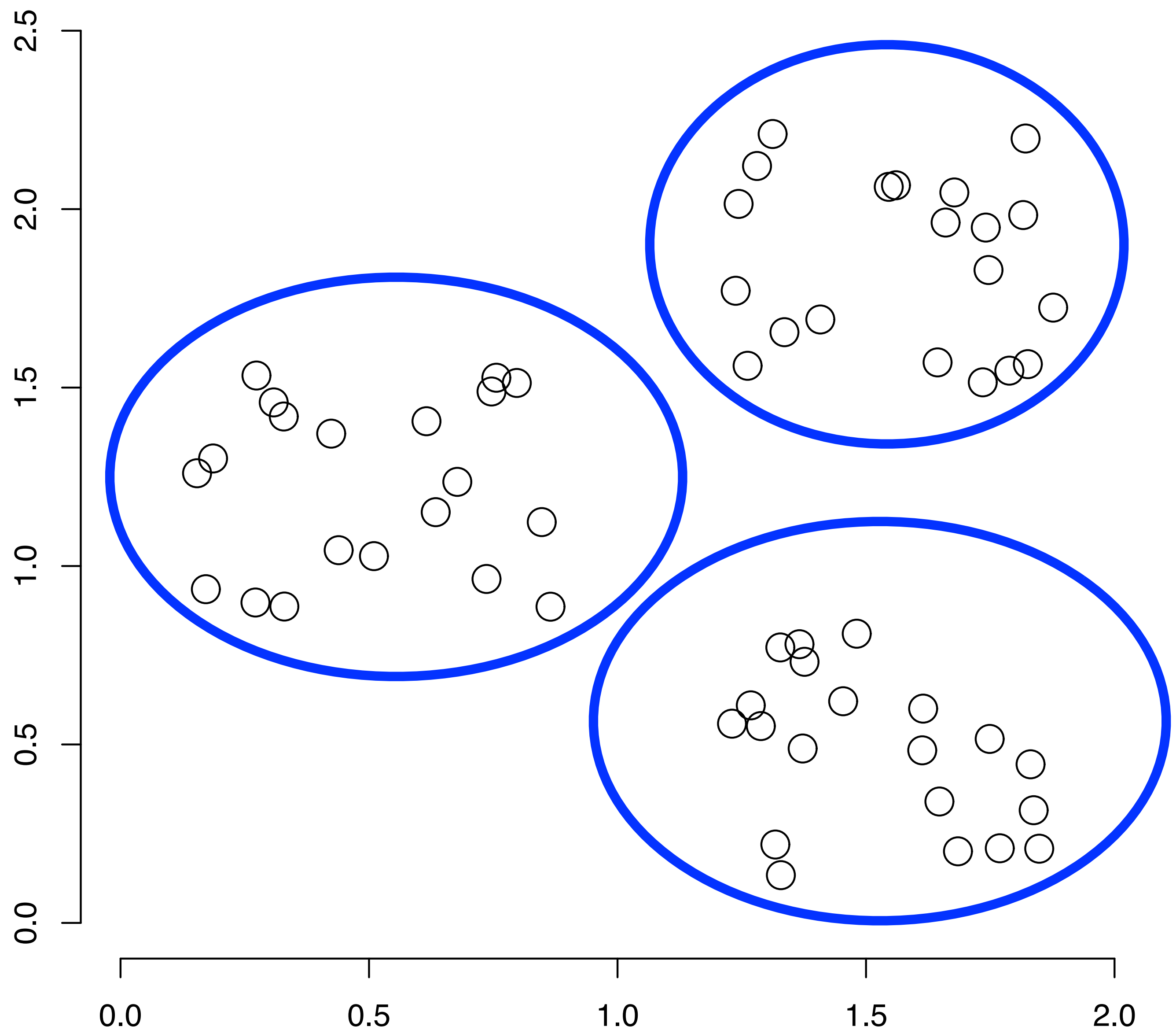
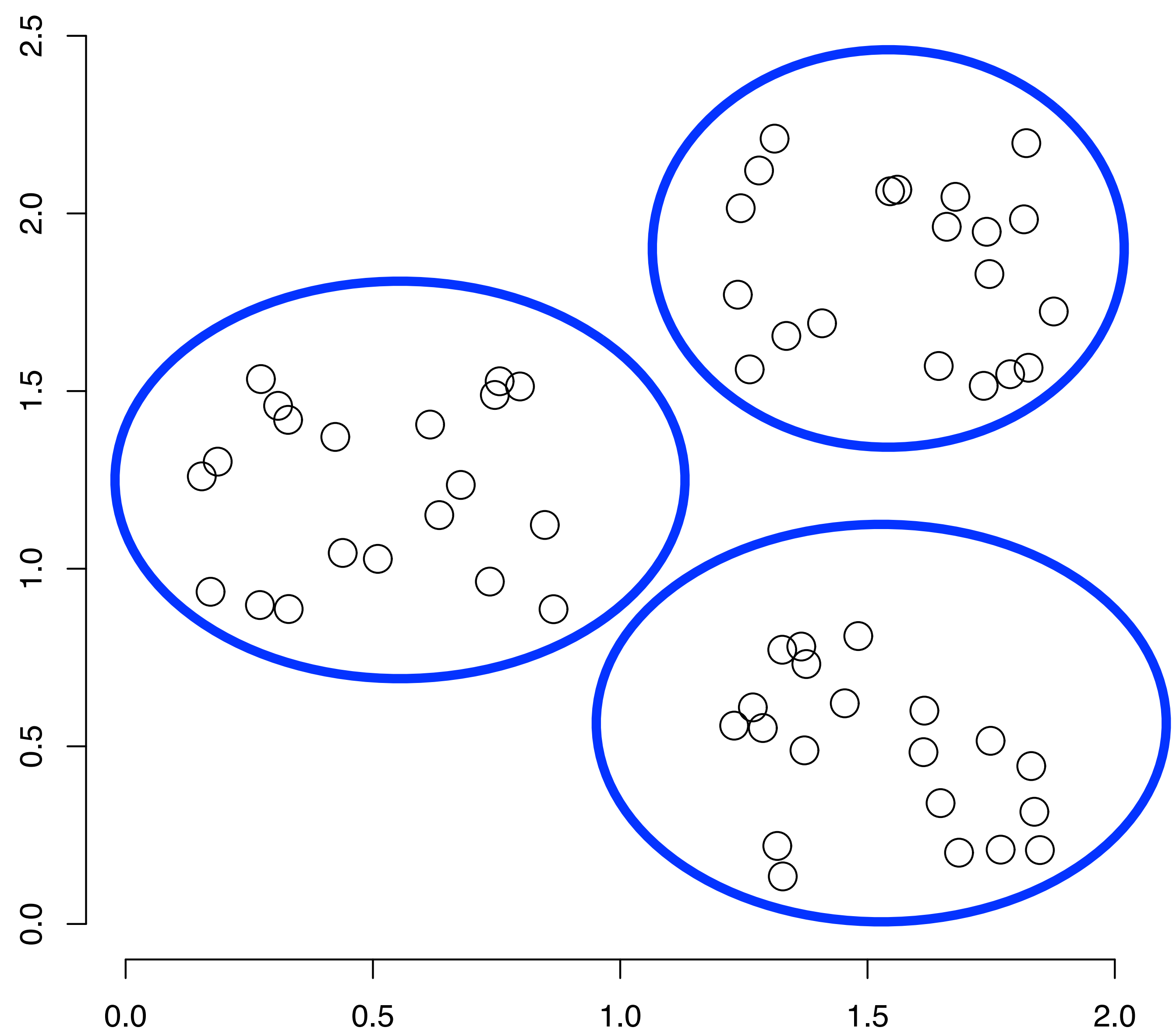


Clustering

- Propose an algorithm that might be able to do this!

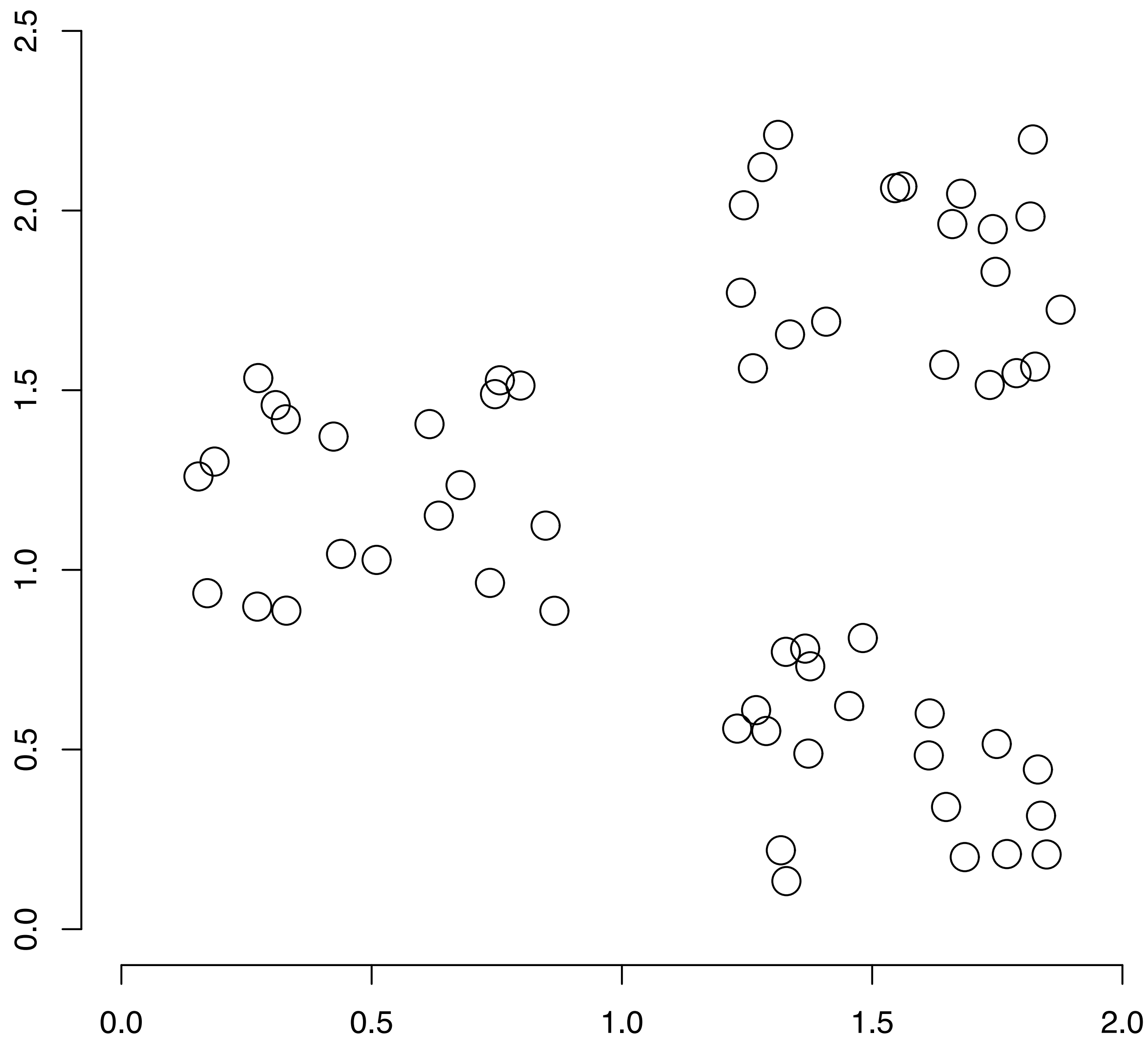


Clustering

- Input: number of desired clusters K
- Output: assignment of documents to K clusters
- Algorithm:
  - randomly select K documents (seeds)
  - assign each remaining document to its nearest seed

Clustering

- Could this work?

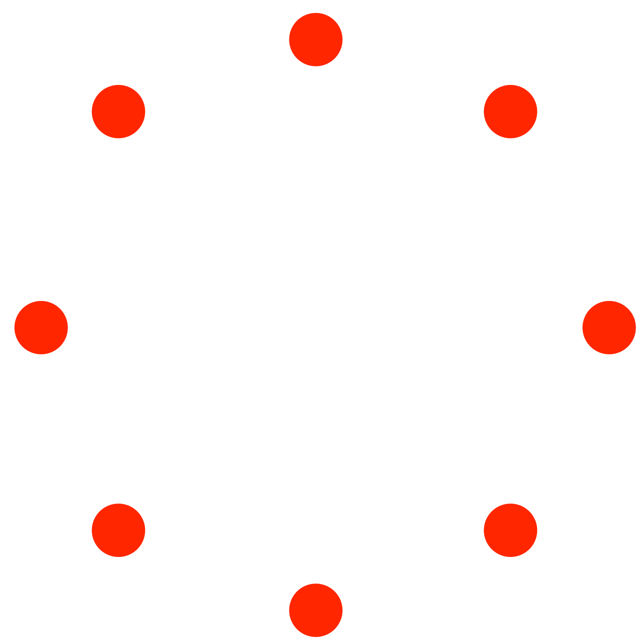


K-Means Clustering

K-means Clustering

cluster centroid

- The key to understanding K-means clustering is to understand the idea of a cluster centroid
- Given a cluster, you can think of its centroid as a point (or vector) that corresponds to its “center of mass”



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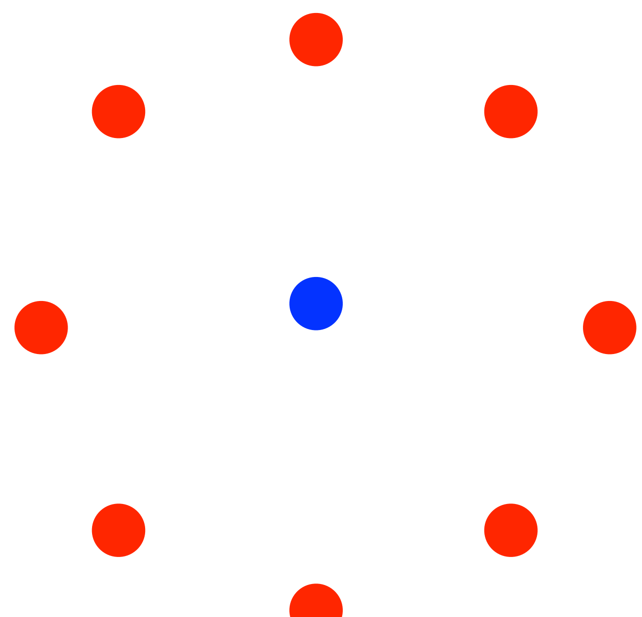

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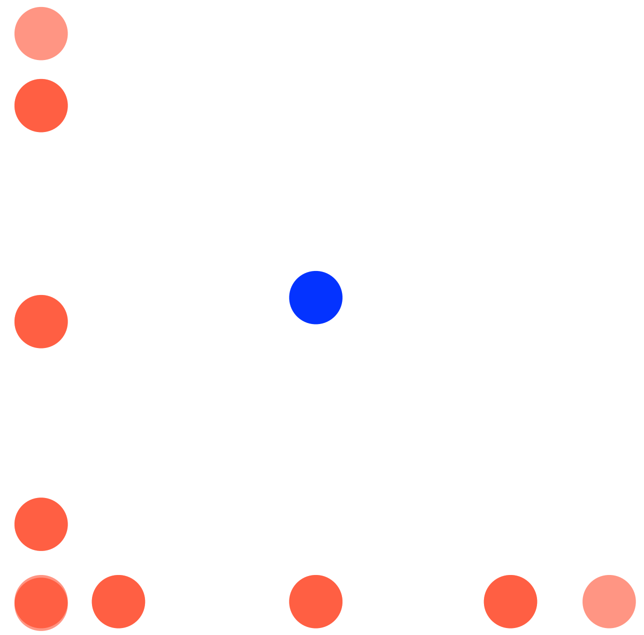

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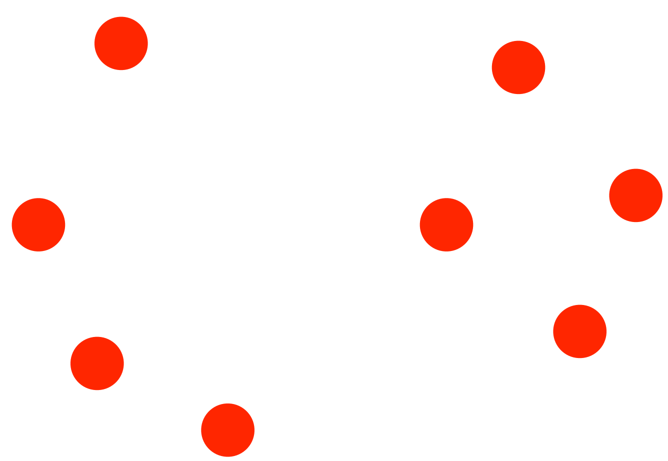

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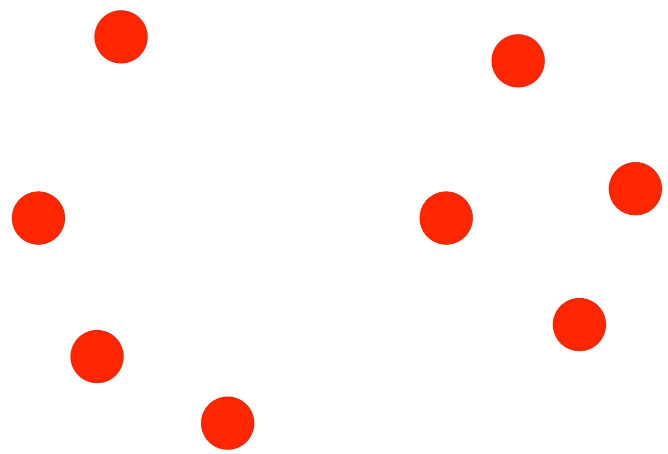

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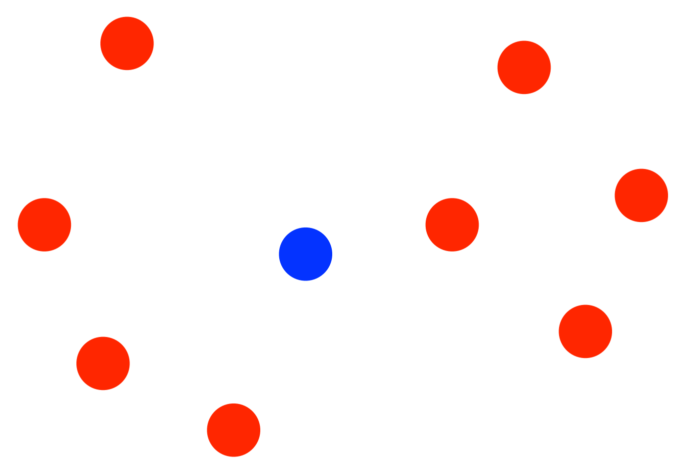

K-means Clustering

cluster centroid

docs assigned to cluster 1

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
1	0	1	0	1	0	0	1	1	0
0	1	0	1	1	0	1	1	0	0
0	1	0	1	1	0	1	0	0	0
0	0	1	0	1	1	0	1	1	1
0	0	1	0	1	1	0	1	1	1
1	1	0	1	1	0	0	1	0	1

cluster 1 centroid

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
?	?	?	?	?	?	?	?	?	?

K-means Clustering

cluster centroid

docs assigned to cluster 1

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
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0	1	0	1	1	0	1	1	0	0
0	1	0	1	1	0	1	0	0	0
0	0	1	0	1	1	0	1	1	1
0	0	1	0	1	1	0	1	1	1
1	1	0	1	1	0	0	1	0	1

cluster 1 centroid (average!)

w_1	w_2	w_3	w_4	w_5	w_6	w_7	w_8	w_9	w_10
0.33	0.50	0.50	0.50	1.00	0.33	0.33	0.83	0.50	0.50

K-means Clustering

cluster centroid

- For each dimension i, set:

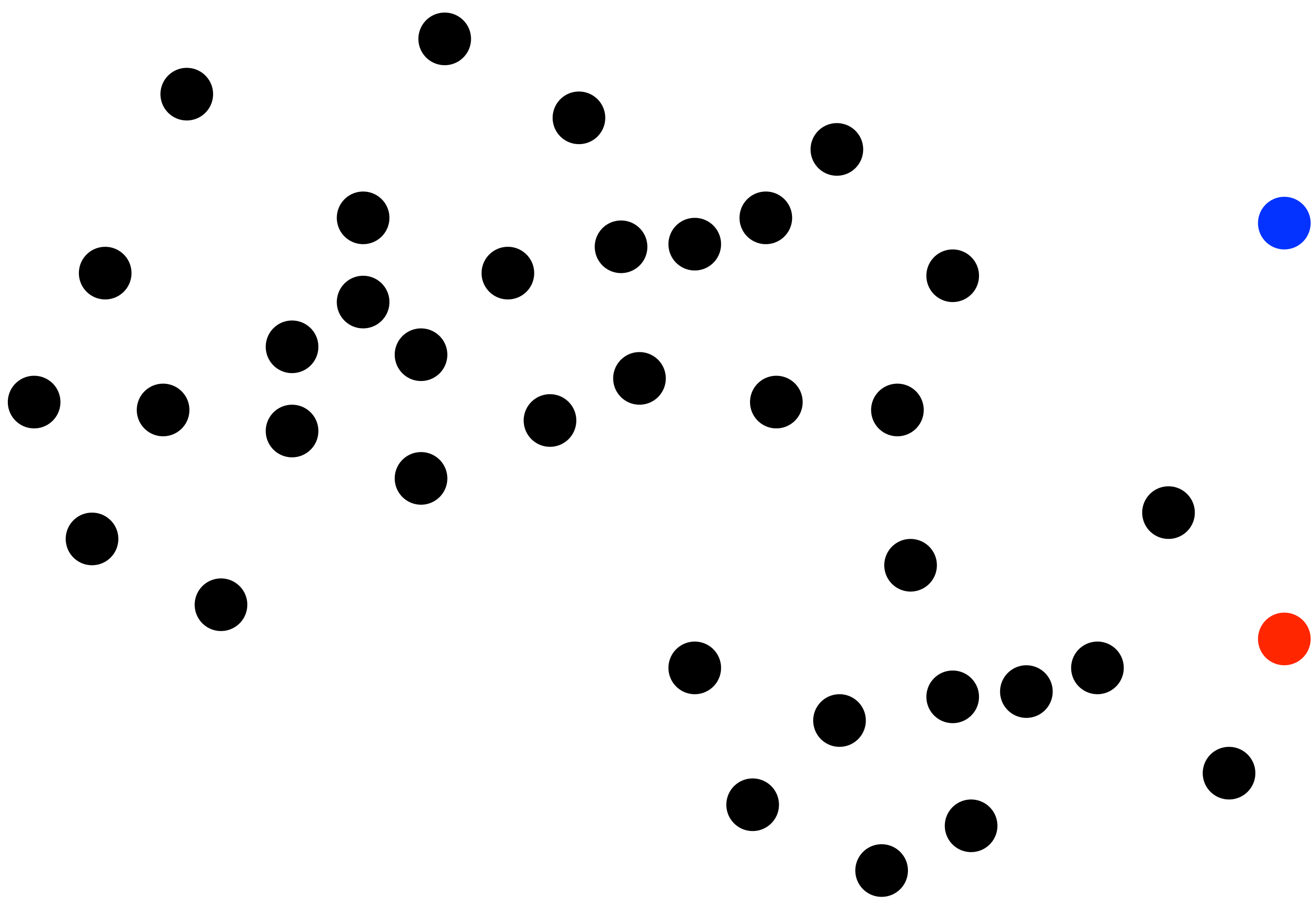
$$c_i = \frac{1}{|C|} \sum_{d \in C} d_i$$

K-means Clustering

- Input: number of desired clusters K
- Output: assignment of documents to K clusters
- Algorithm:
  - Step 1: randomly select K documents (seeds)
  - Step 2: assign each document to its nearest seed
  - Step 3: compute all K cluster centroids
  - Step 4: re-assign each document to its nearest centroid
  - Step 5: re-compute all K cluster centroids
  - Step 6: repeat steps 4 and 5 until terminating condition

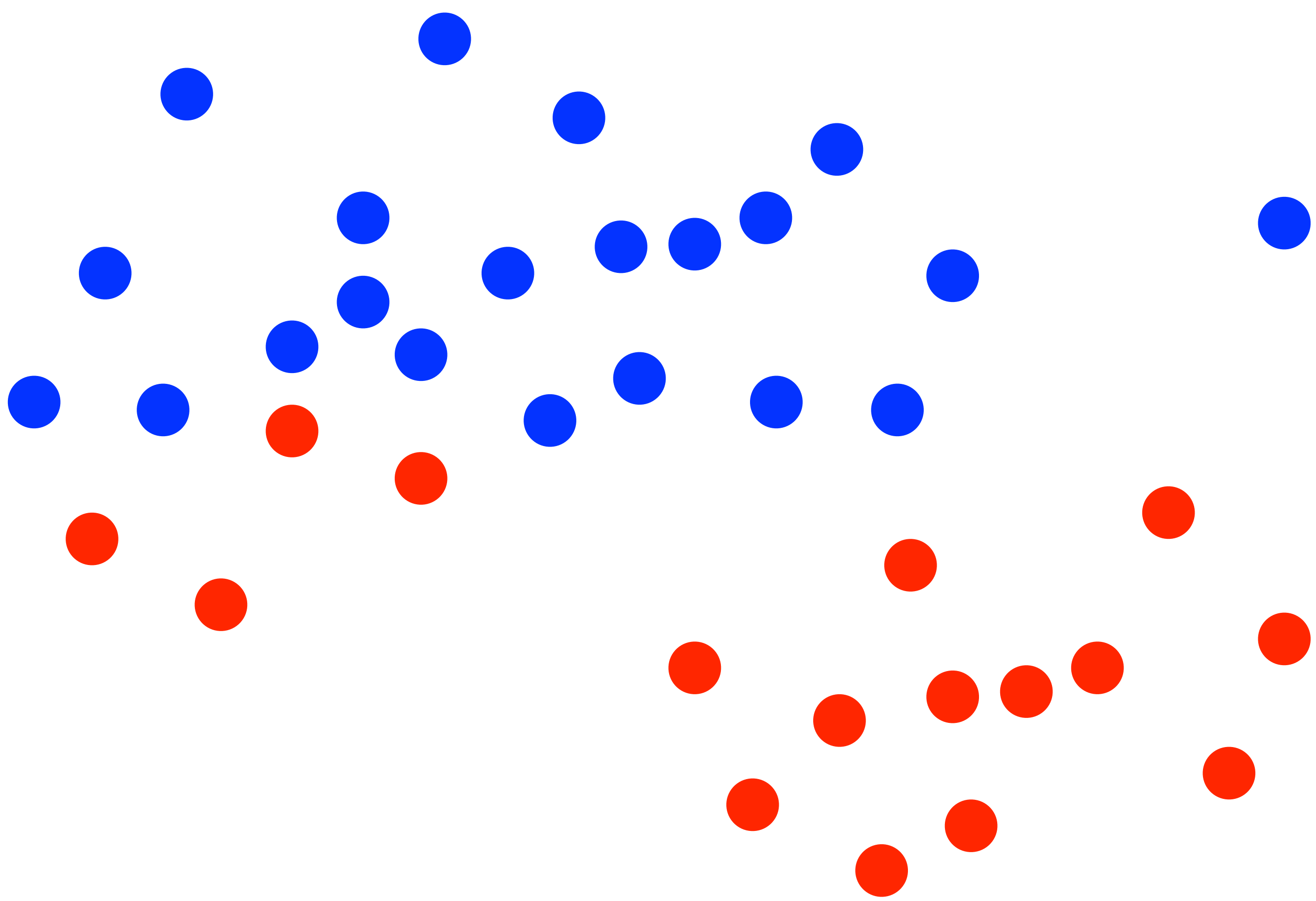
K-means Clustering

- Step 1: randomly select K documents (seeds)



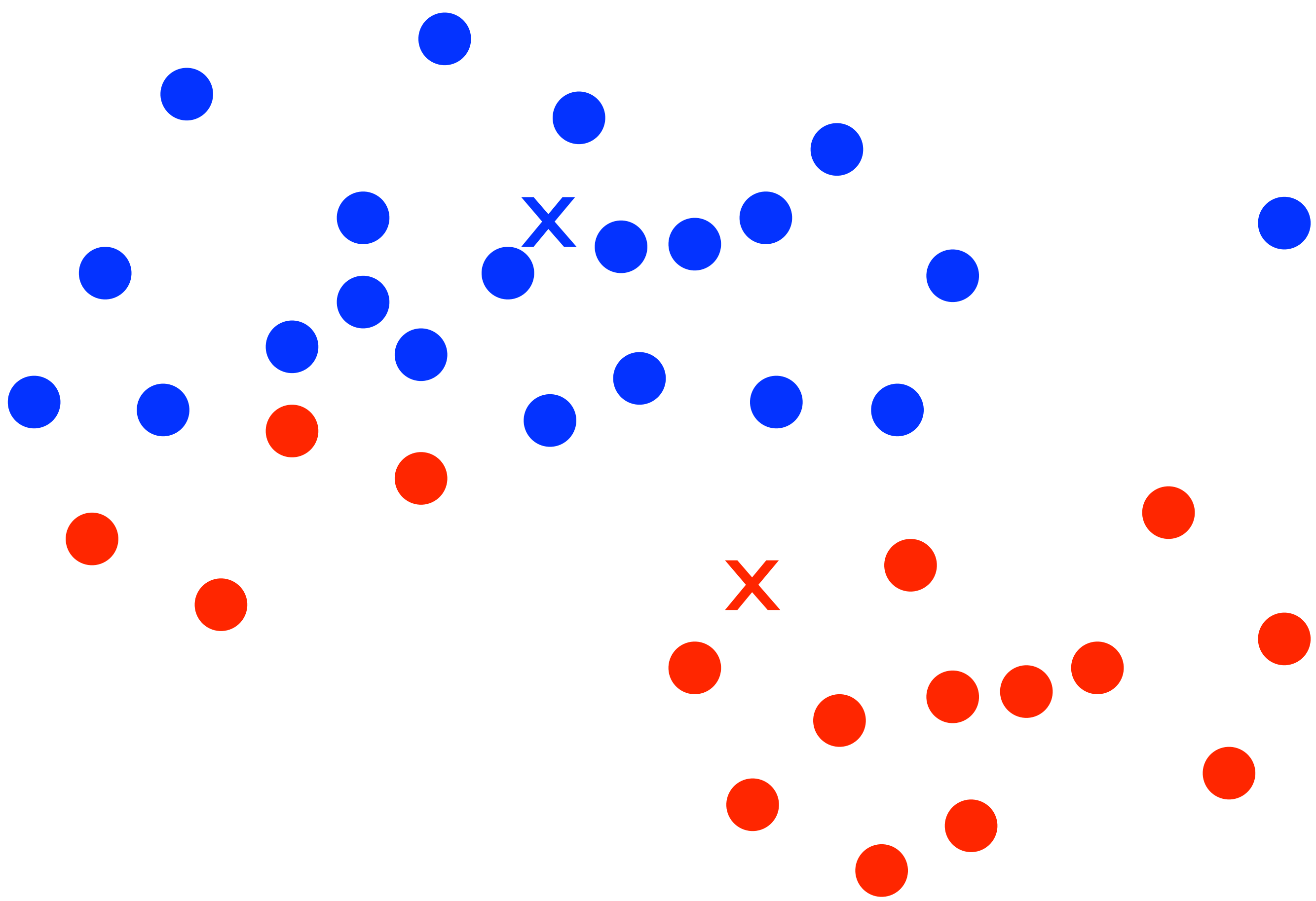
K-means Clustering

- Step 2: assign each document to its nearest seed



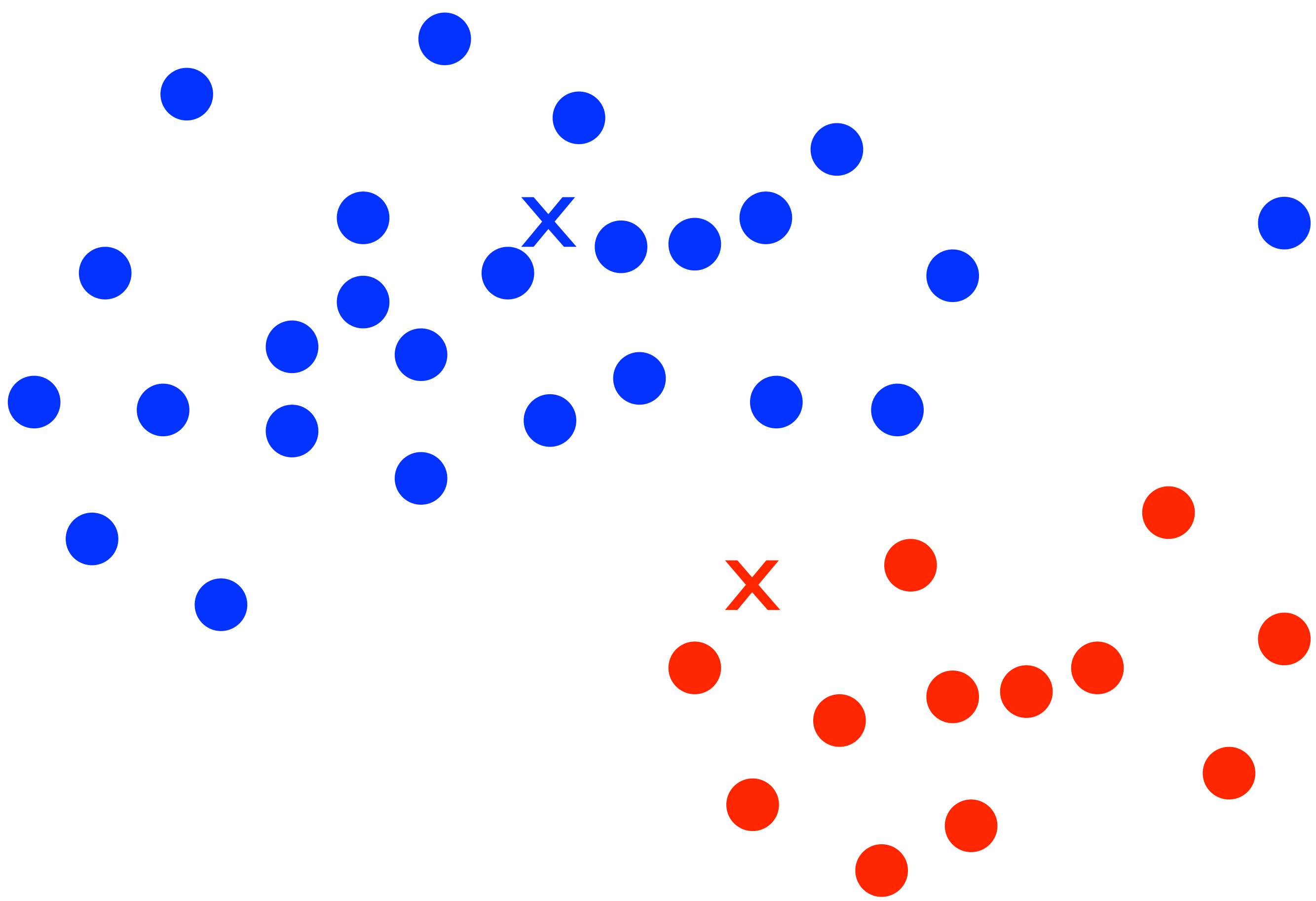
K-means Clustering

- Step 3: compute all K cluster centroids



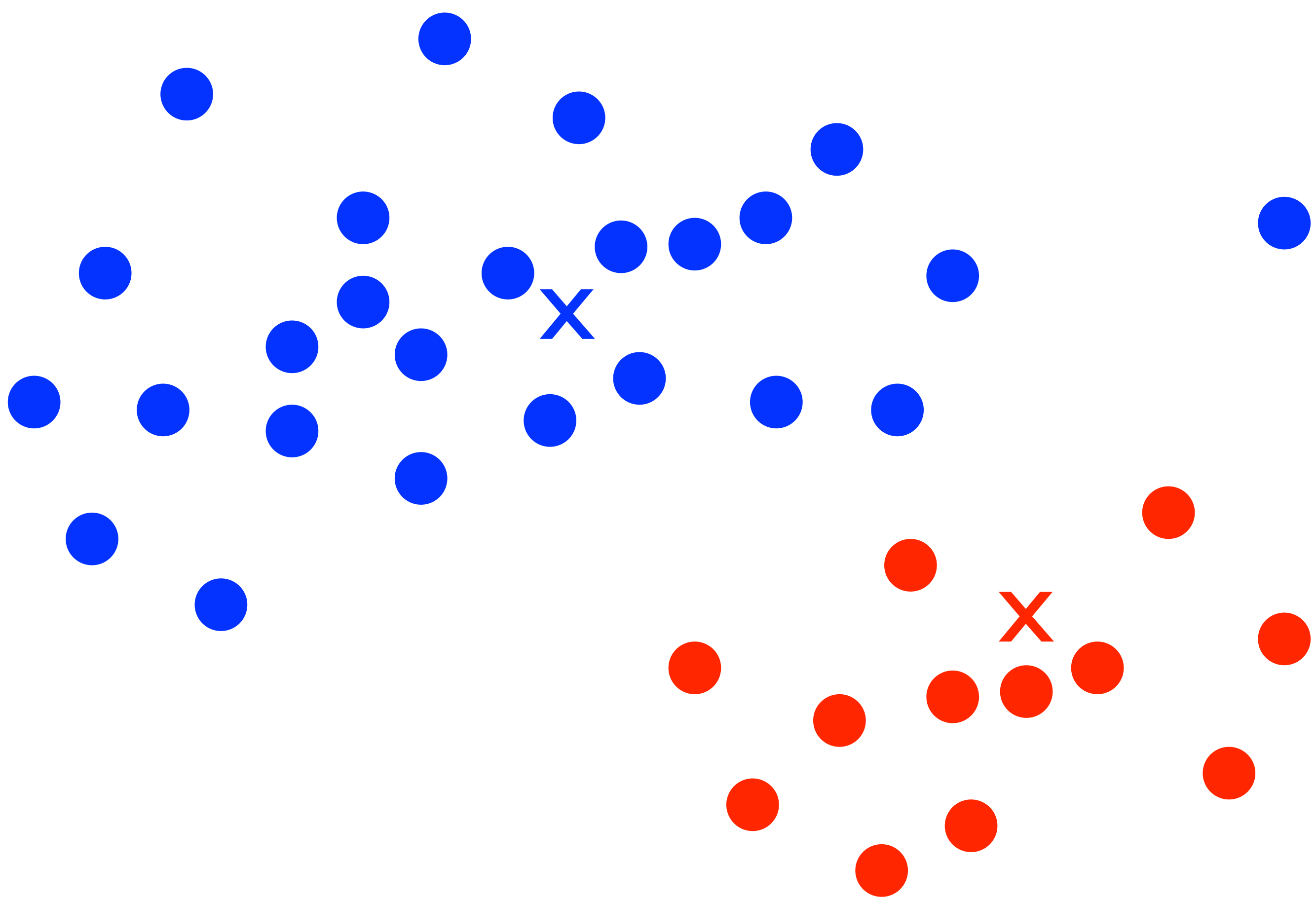
K-means Clustering

- Step 4: re-assign each document to its nearest centroid



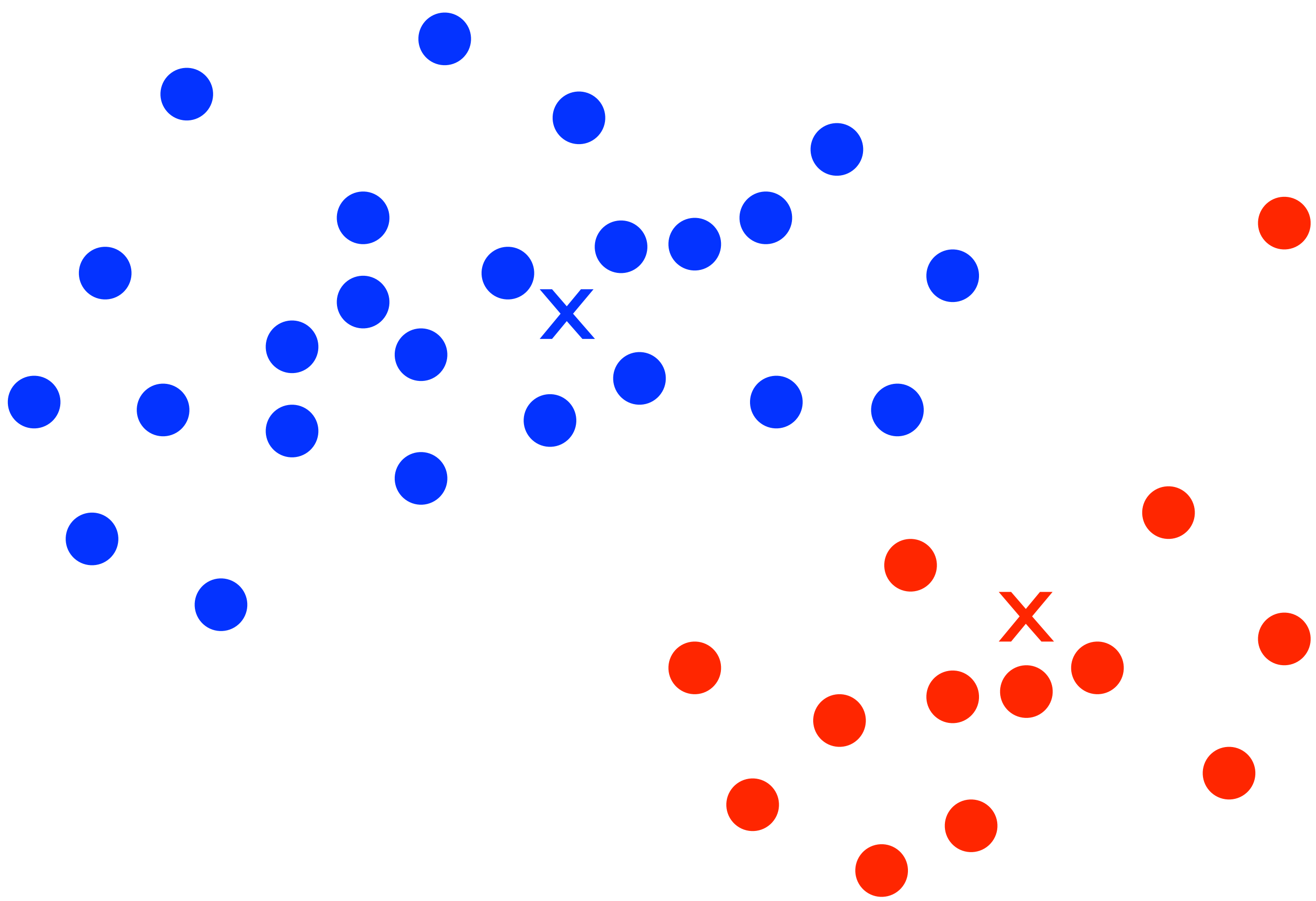
K-means Clustering

- Step 4: re-compute all K cluster centroids



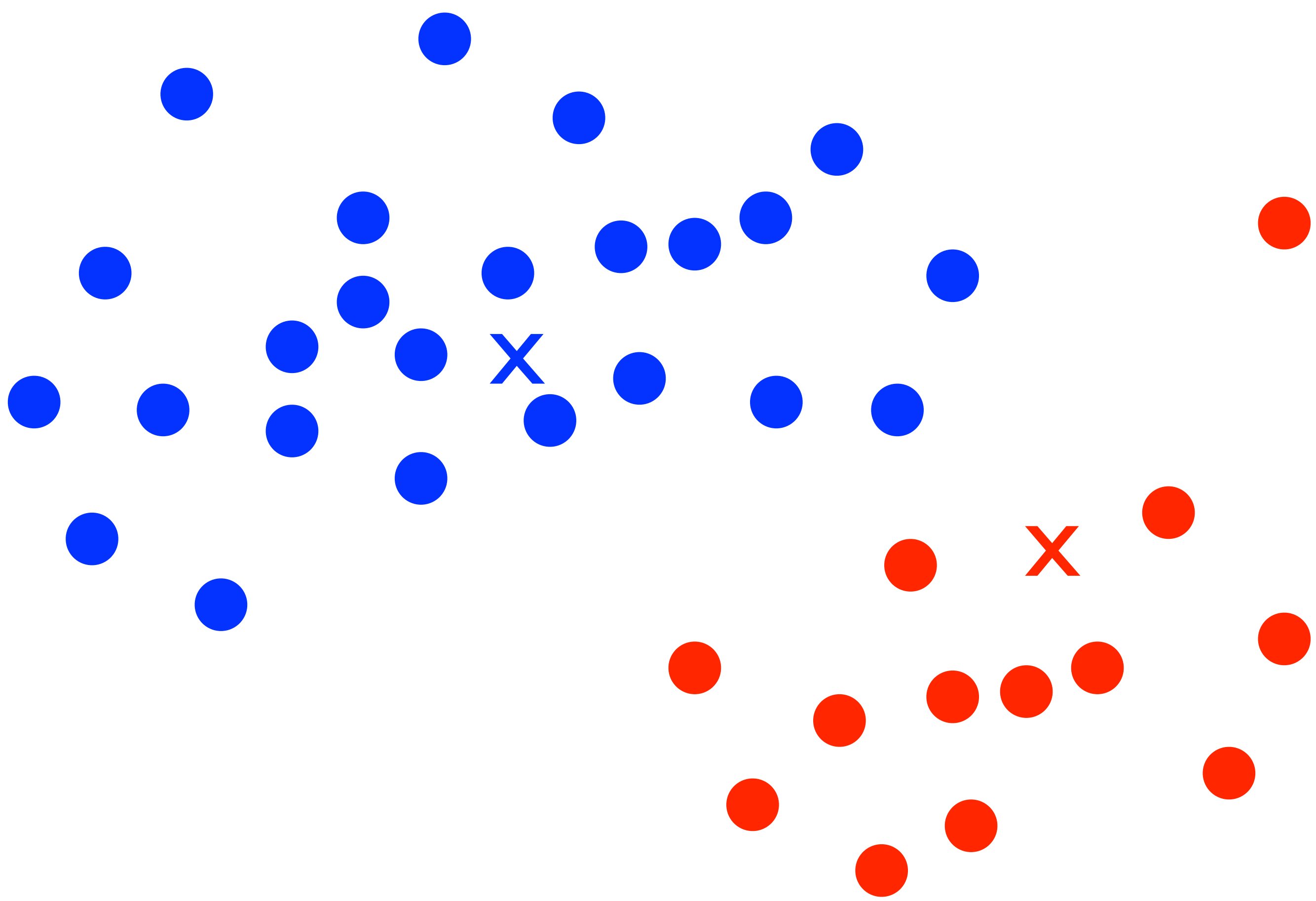
K-means Clustering

- Step 5: re-assign each document to its nearest centroid



K-means Clustering

- Step 4: re-compute all K cluster centroids



K-means Clustering

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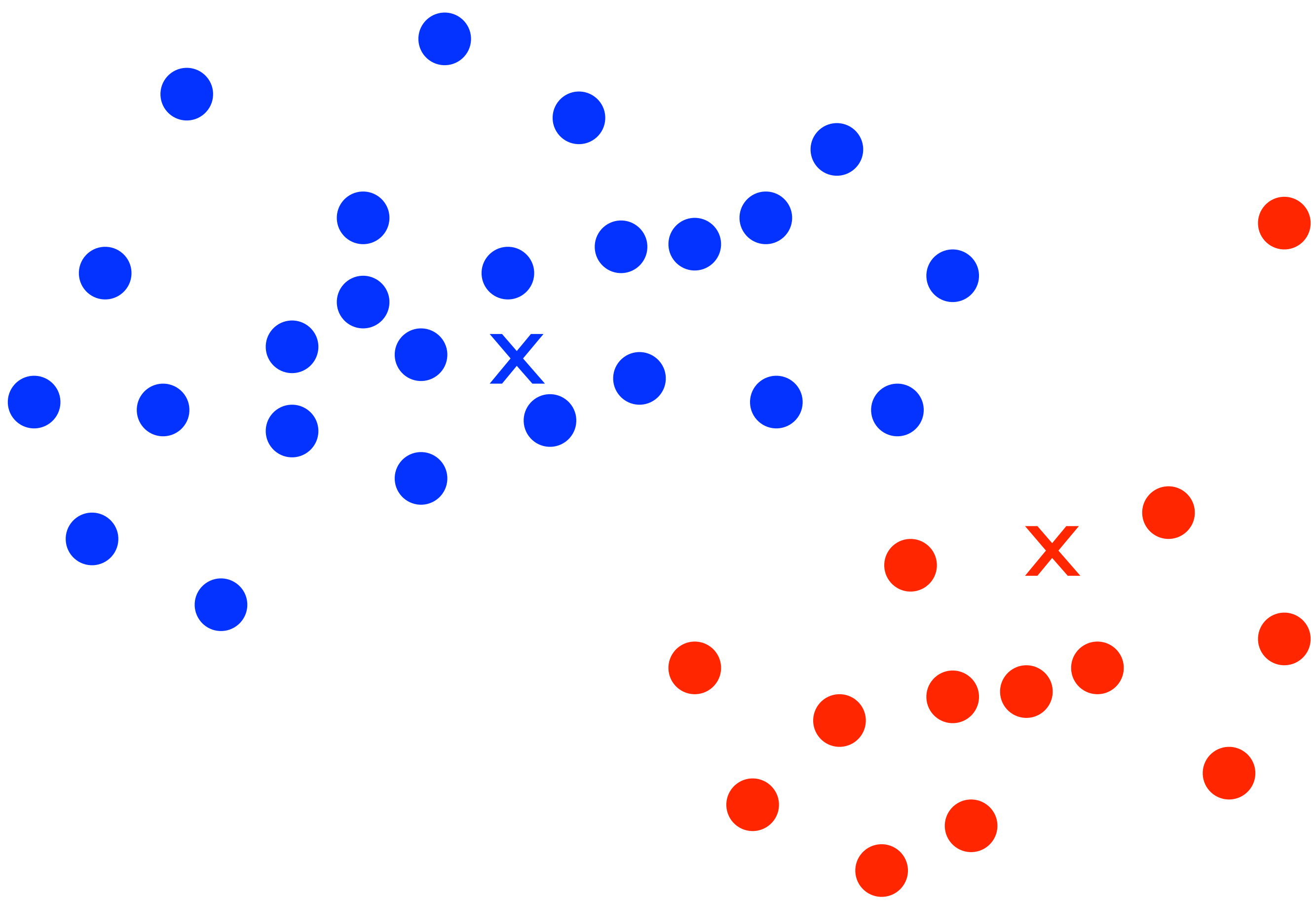

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  - Step 6: repeat steps 4 and 5 until terminating condition

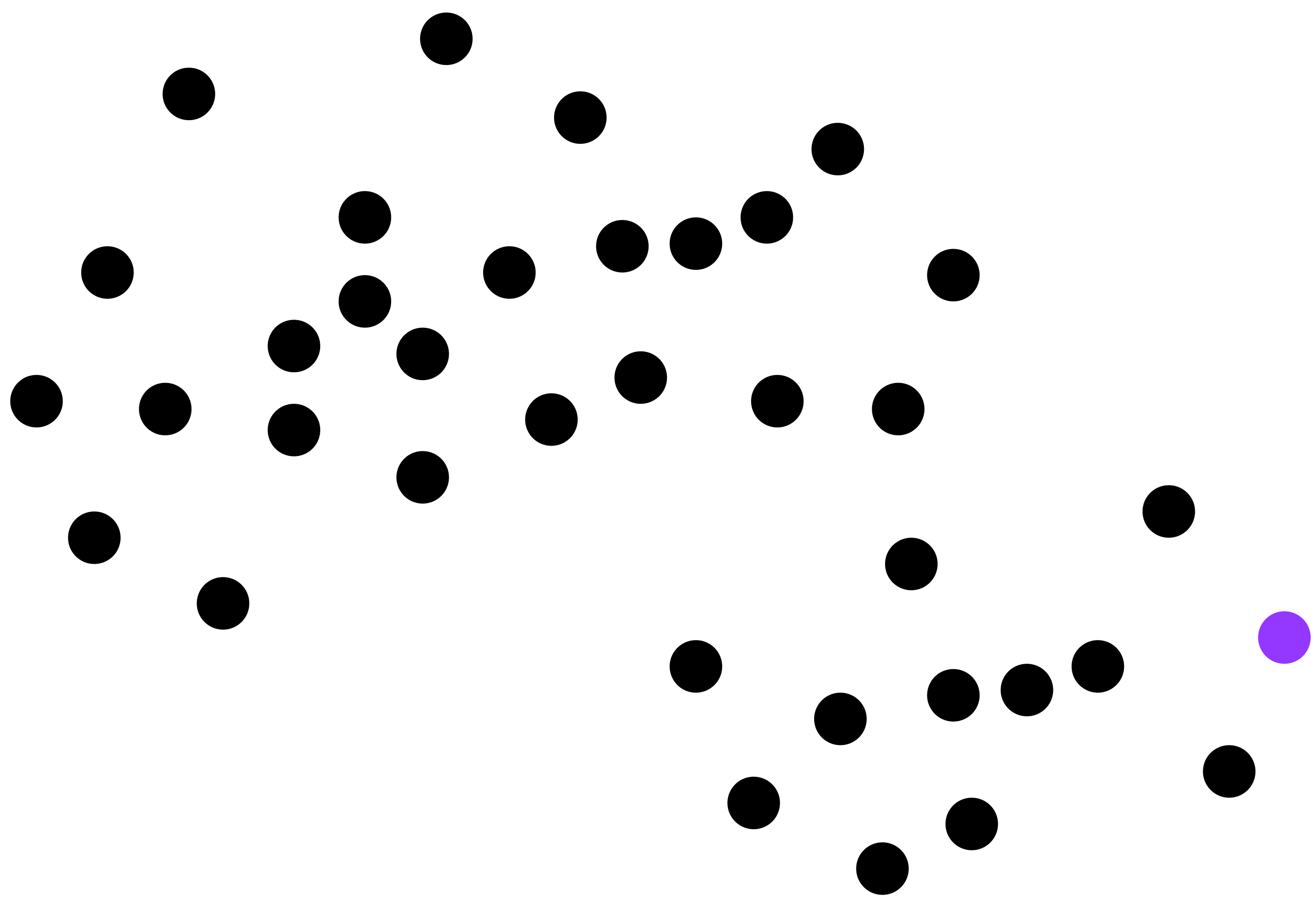
K-means Clustering

potential drawback

- The quality of the output clustering depends on the choice of K and on the initial seeds
- In many cases, the choice of K is pre-determined by the application
  - Search engine results clustering: grouping search engine results by topic
  - Collection clustering: grouping documents by topic to support navigation and exploration
- Later we'll see ways of setting K dynamically

K-means Clustering

bad seeds?



K-means Clustering

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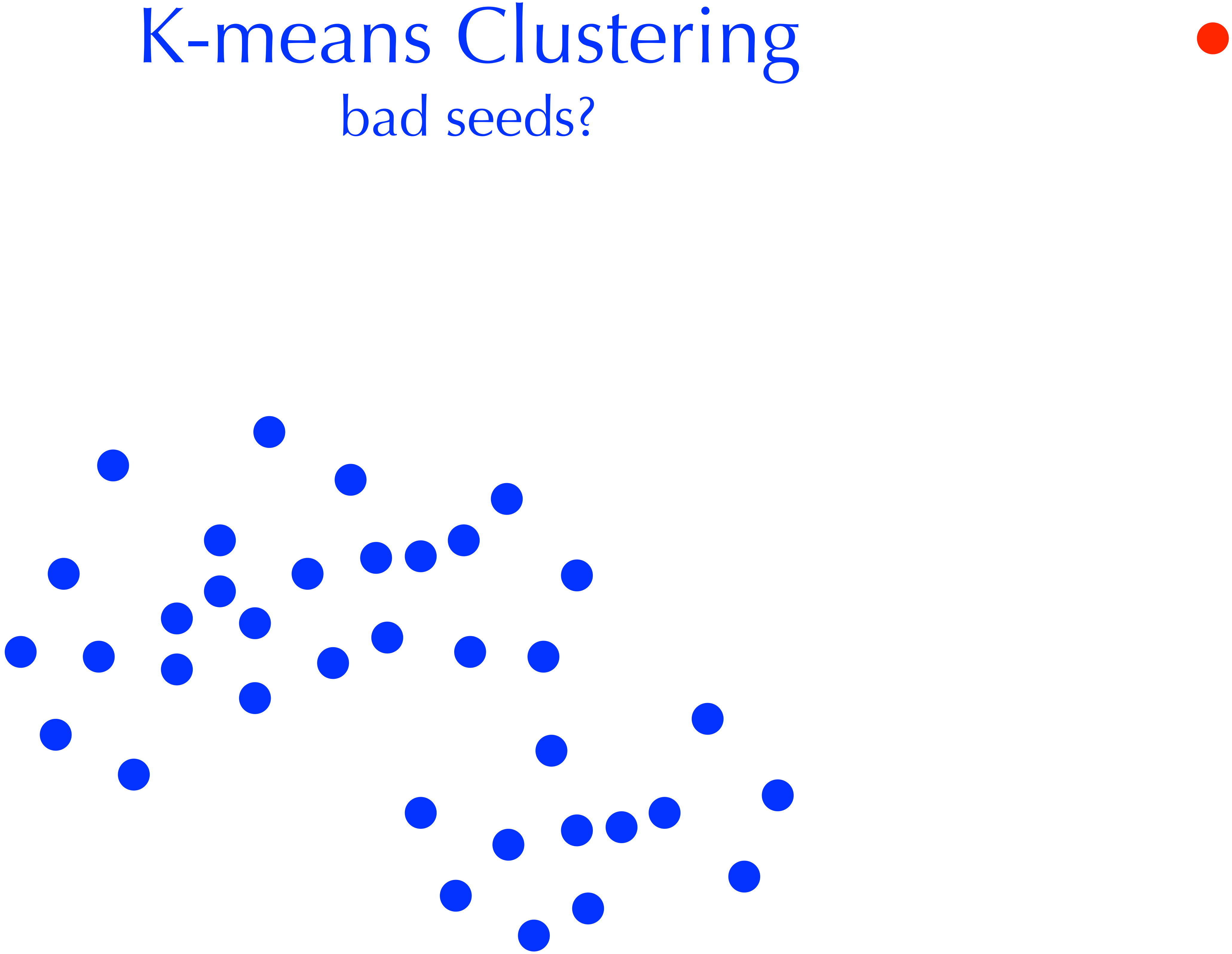

K-means Clustering

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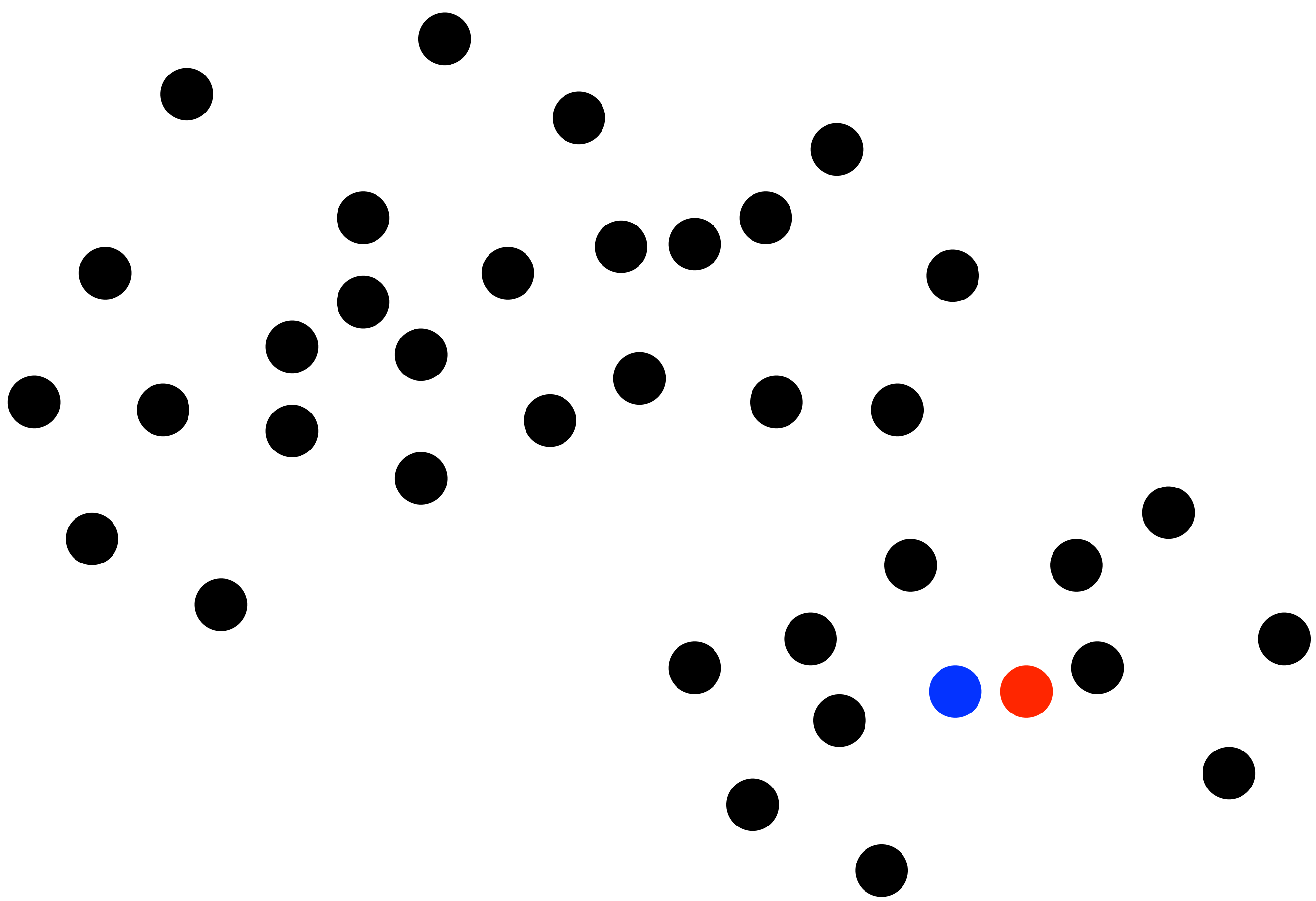
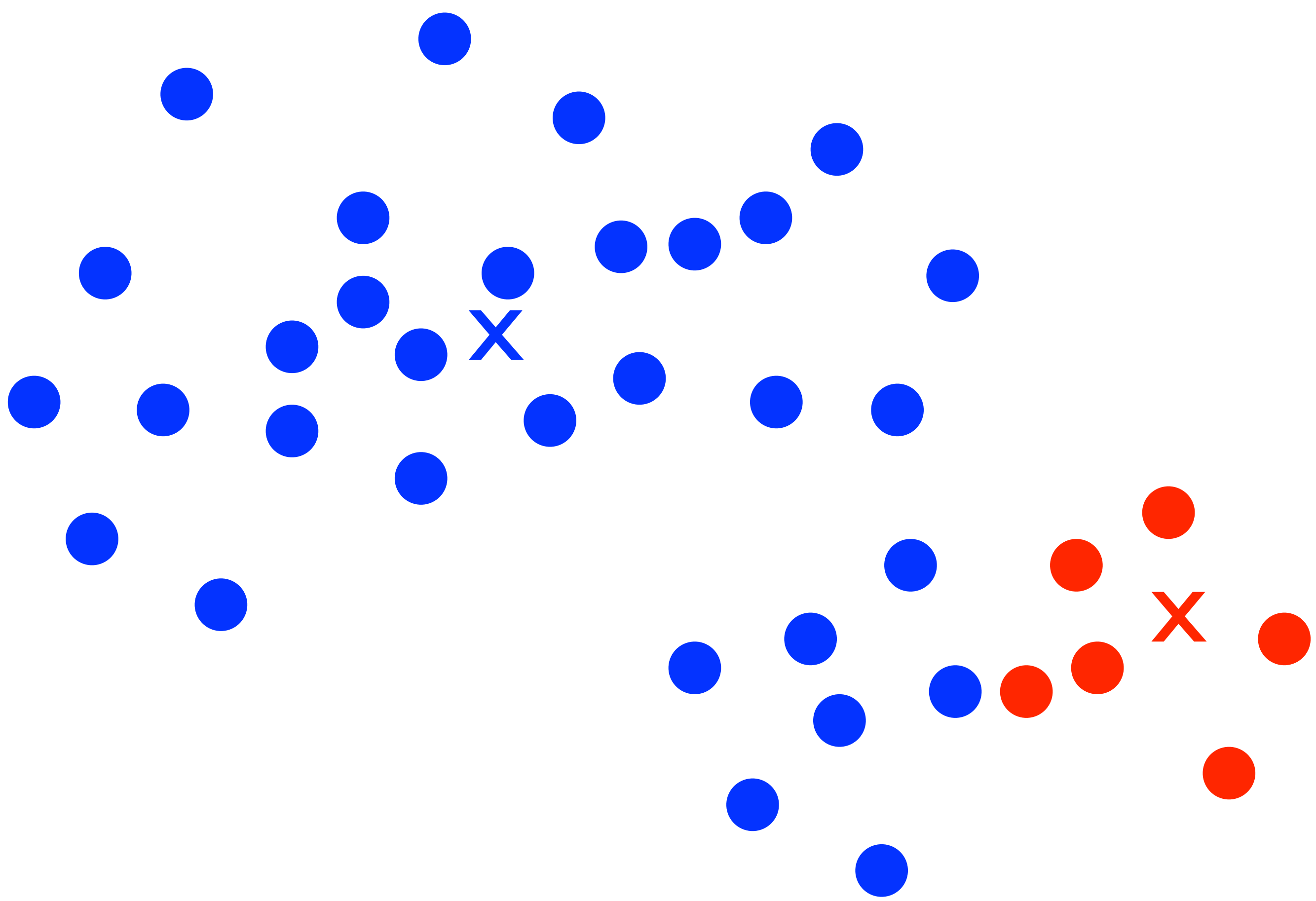


K-means Clustering
bad seeds?



K-means Clustering
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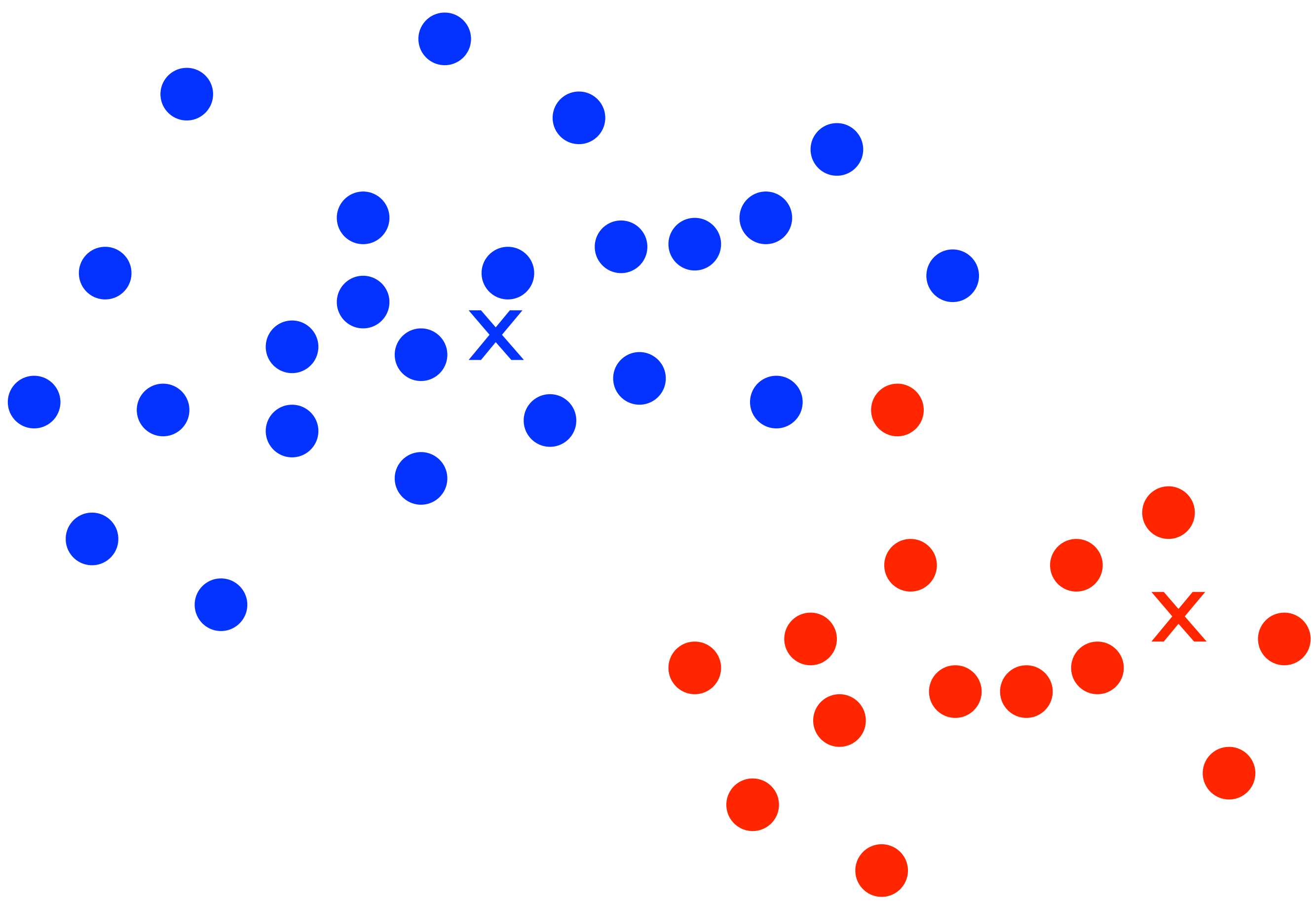

K-means Clustering
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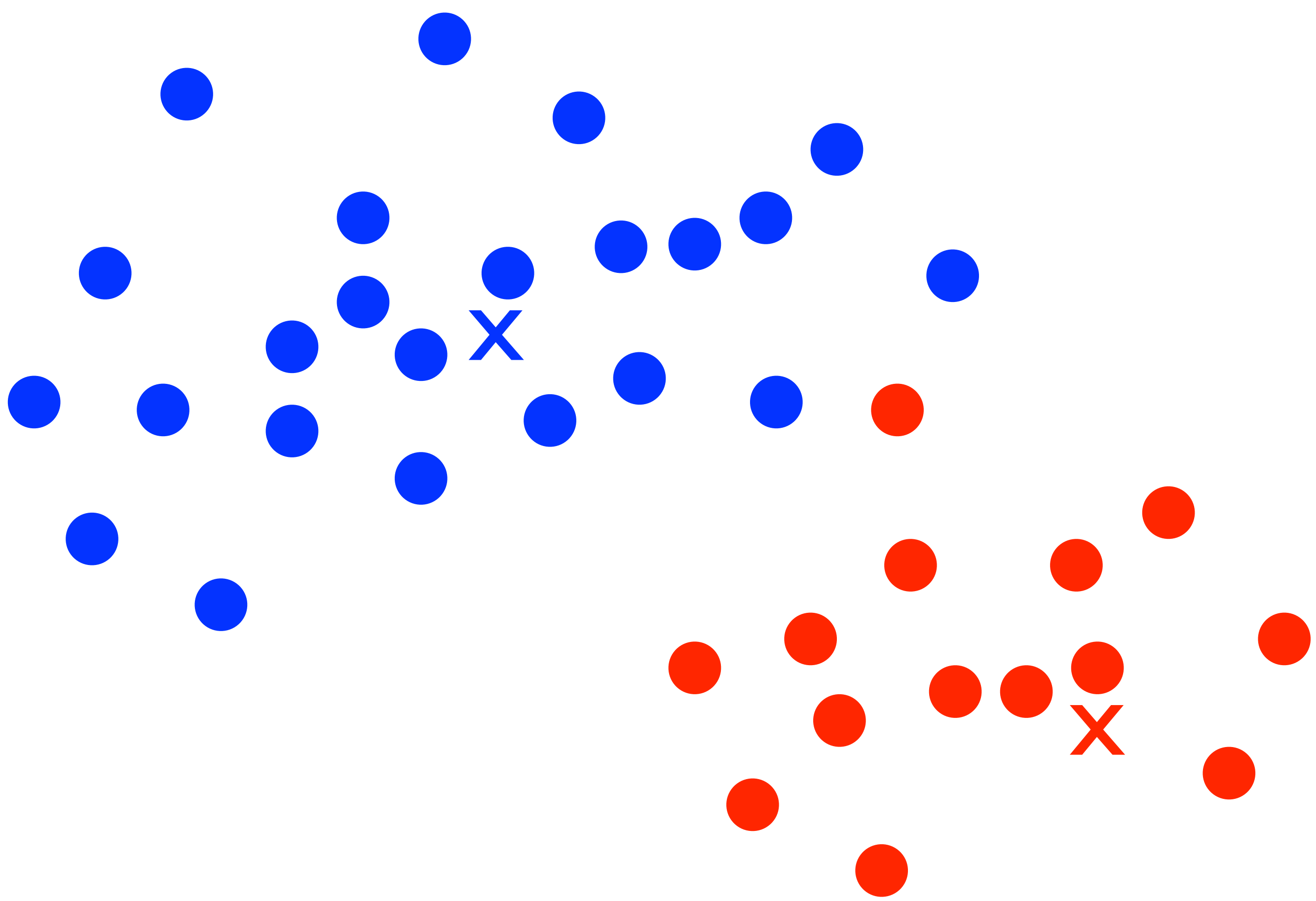
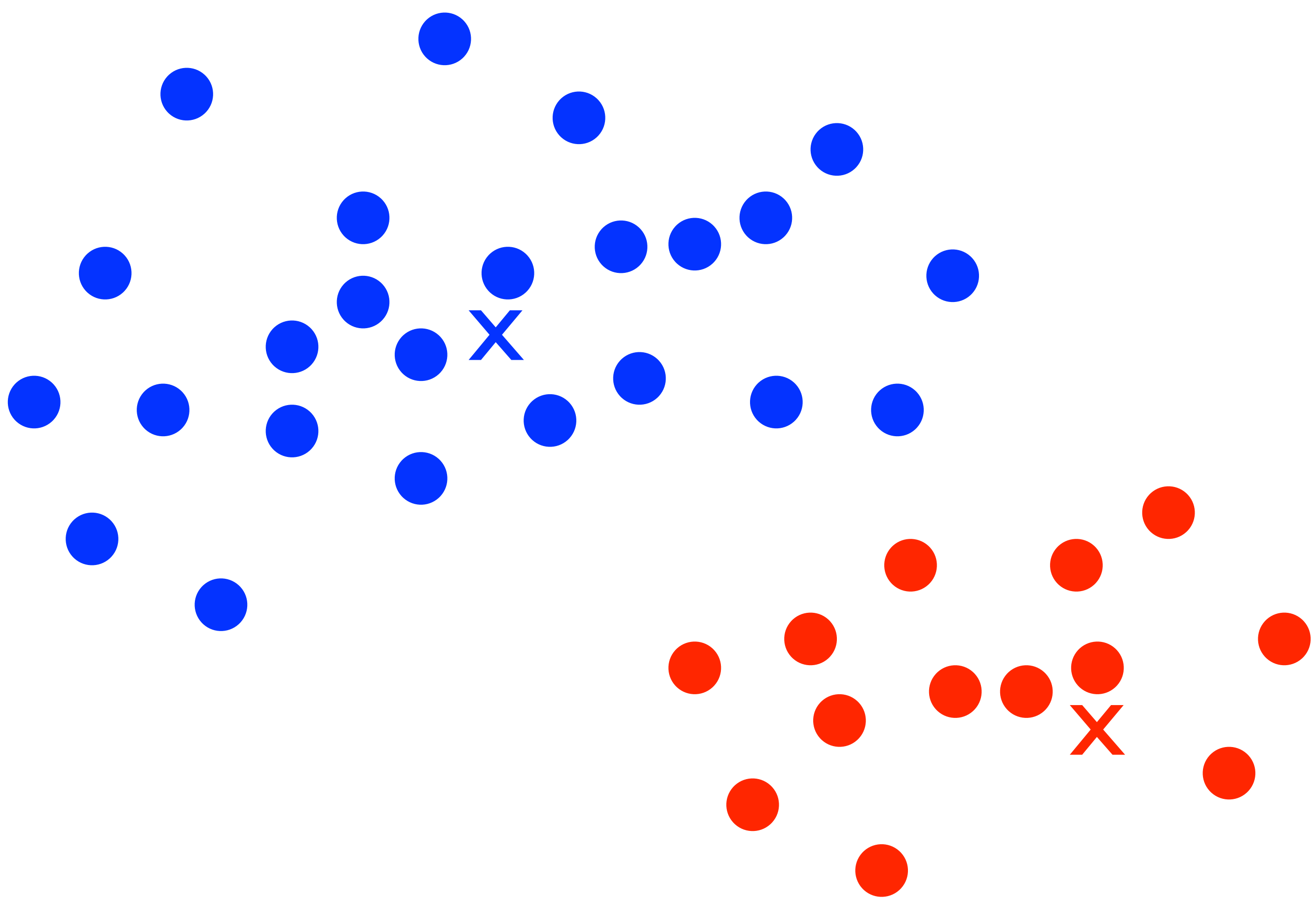


K-means Clustering

bad seeds?



K-means Clustering
bad seeds

- It's difficult to know which seeds will yield a high-quality clustering
- However, it's usually a good idea to avoid seeds that are outliers
- How would you detect outliers?

K-means Clustering
clustering evaluation

- What does it mean for a clustering to be high quality anyway?
- What is the goal of clustering again?

K-means Clustering
internal evaluation

- In theory, a good clustering should have:
  - Similar documents in the same clusters
  - Different documents in different clusters

K-means Clustering

internal evaluation

$$\text{Clustering Quality} = \left(\begin{array}{c} \text{Average distance} \\ \text{between all pairs} \\ \text{of documents in} \\ \underline{\text{different clusters}} \end{array} \right) - \left(\begin{array}{c} \text{Average distance} \\ \text{between all pairs of} \\ \text{documents in the} \\ \underline{\text{same cluster}} \end{array} \right)$$

K-means Clustering
improved k-means

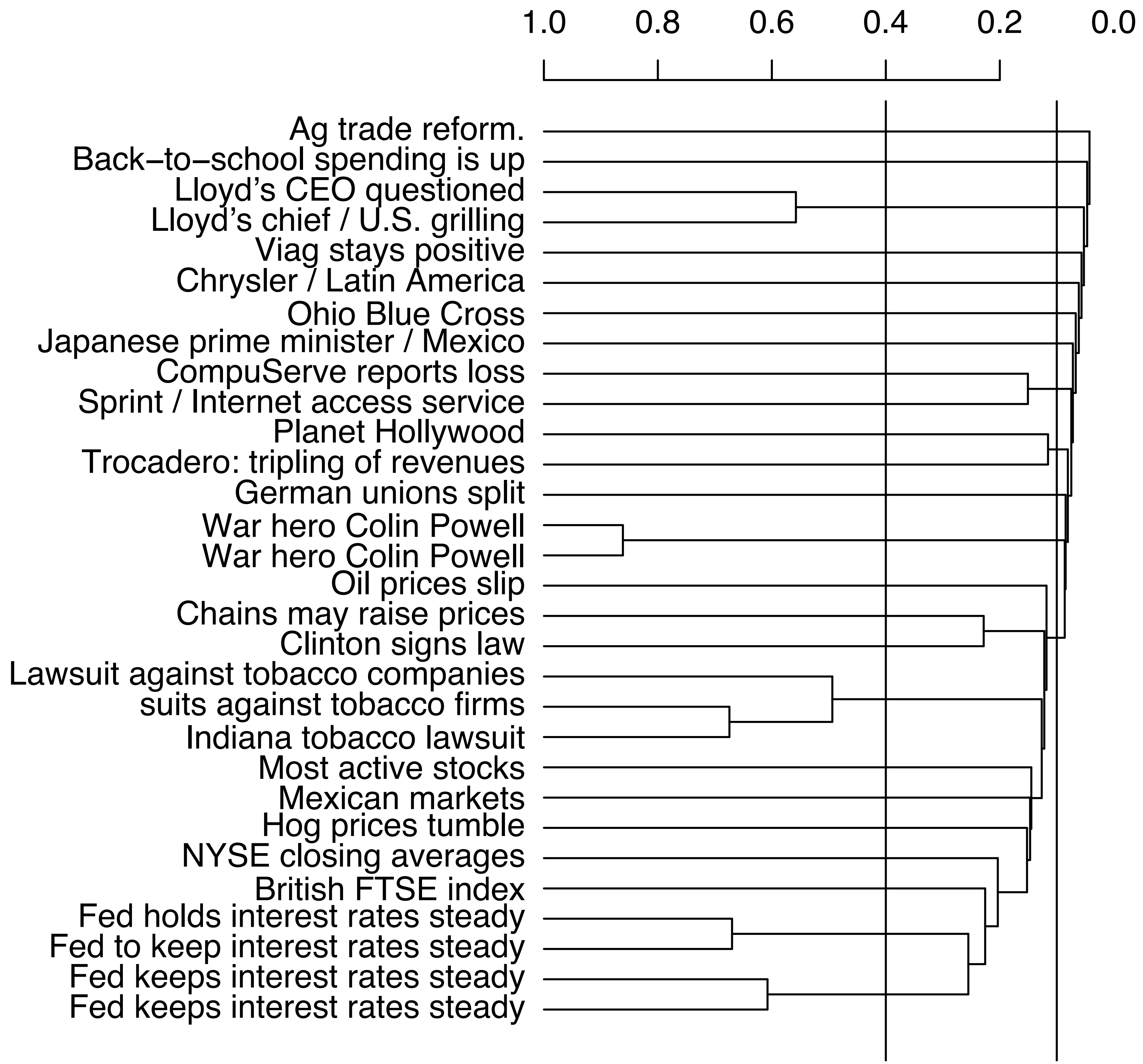
- Given a set of documents and a value K, run K-means clustering N times and keep the clustering that produces the greatest difference between the inter-cluster distance and the intra-cluster distance

Bottom-up Agglomerative Clustering

Bottom-up Clustering

- While K-means requires setting K, bottom-up clustering groups the data in a hierarchical fashion
- We can then set K after the clustering is done or use a distance threshold to set K dynamically (more on this later)

Bottom-up Clustering



Bottom-up Clustering

- Input: data
- Output: cluster hierarchy
- Algorithm:
  - Step 1: consider every document its own cluster
  - Step 2: compute the distance between all cluster pairs
  - Step 3: merge/combine the nearest two clusters into one
  - Step 4: repeat steps 2 and 3 until every document is in one cluster

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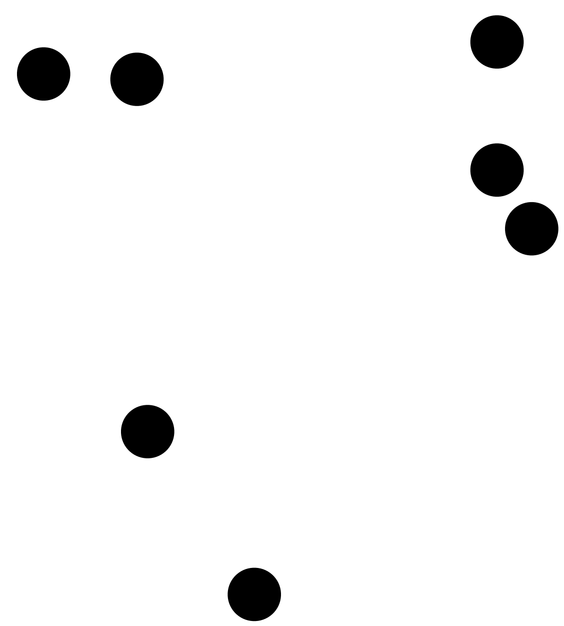
Bottom-up Clustering

- Computing the distance between two clusters
- Single-Link: the distance between the two nearest documents
- Complete-Link: the distance between the two documents that are farthest apart
- Average-Link: the average distance between all document pairs (excluding those in the same cluster)
  - this is equivalent to using the distance between the two cluster centroids

Bottom-up Clustering

single-link

- Step 1: consider each document its own cluster



Bottom-up Clustering
single-link

- Step 2: compute the distance between all cluster pairs
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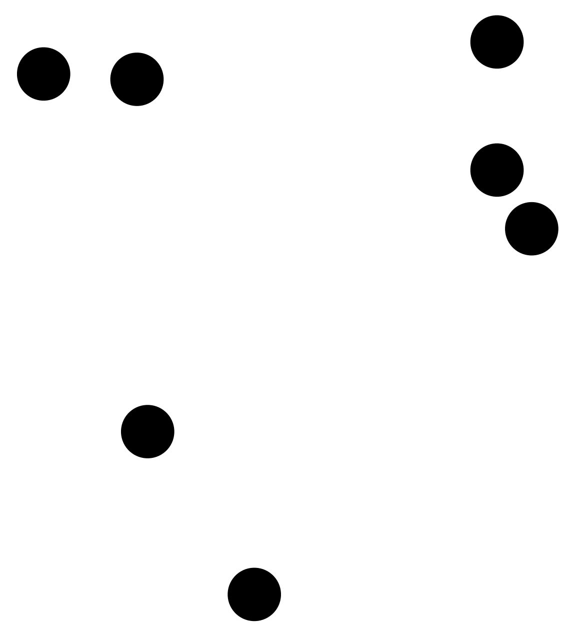
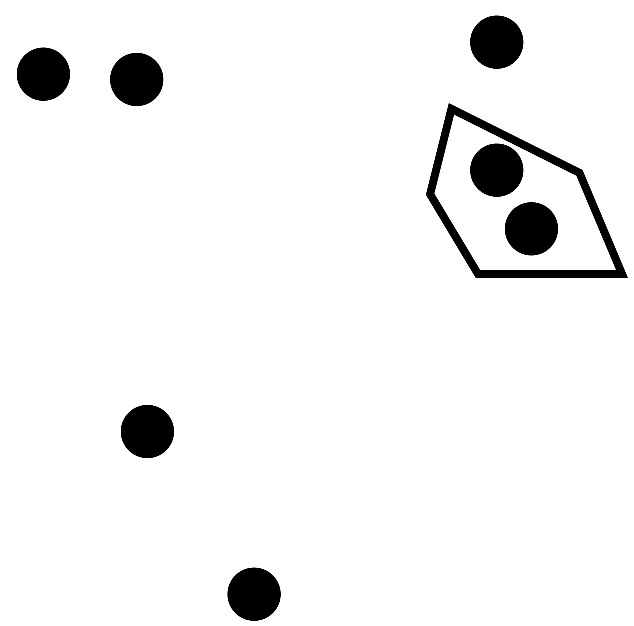


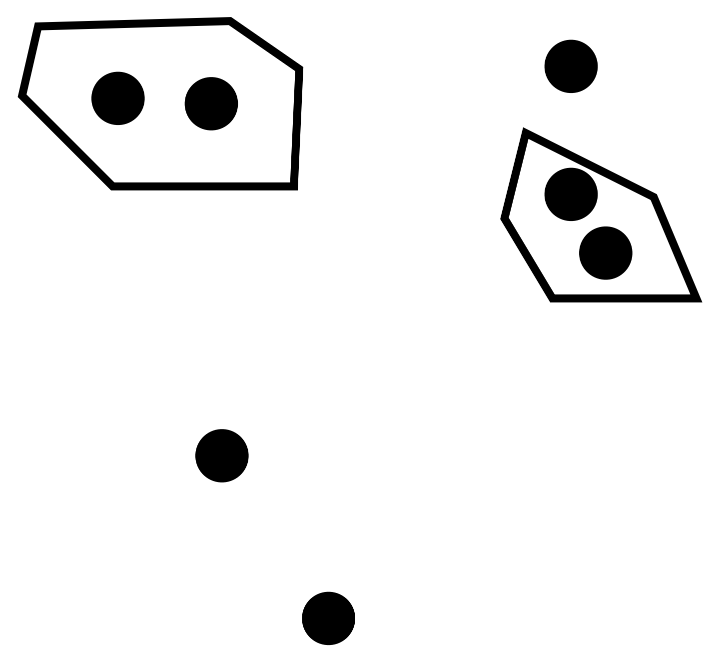
Bottom-up Clustering
single-link

- Step 2: compute the distance between all cluster pairs
- Step 3: merge/combine the nearest two clusters into one



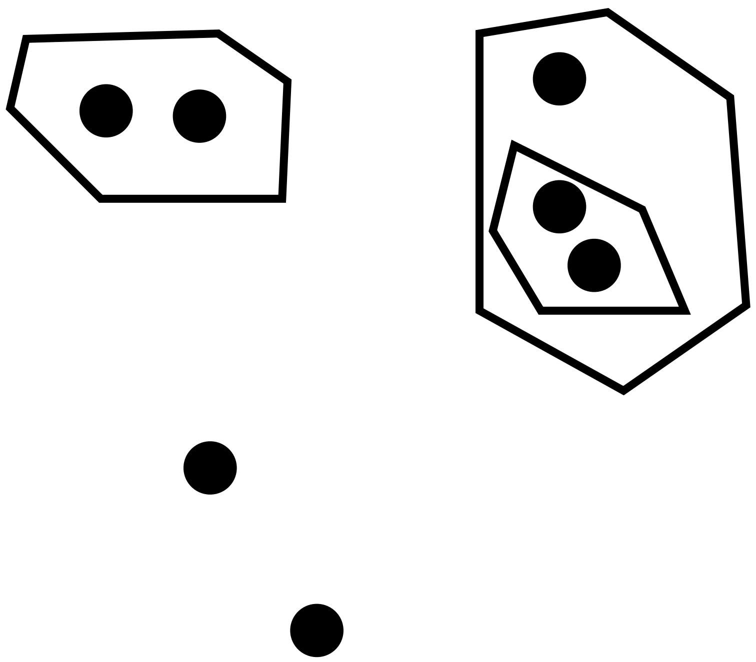
Bottom-up Clustering
single-link

- Step 2: compute the distance between all cluster pairs
- Step 3: merge/combine the nearest two clusters into one



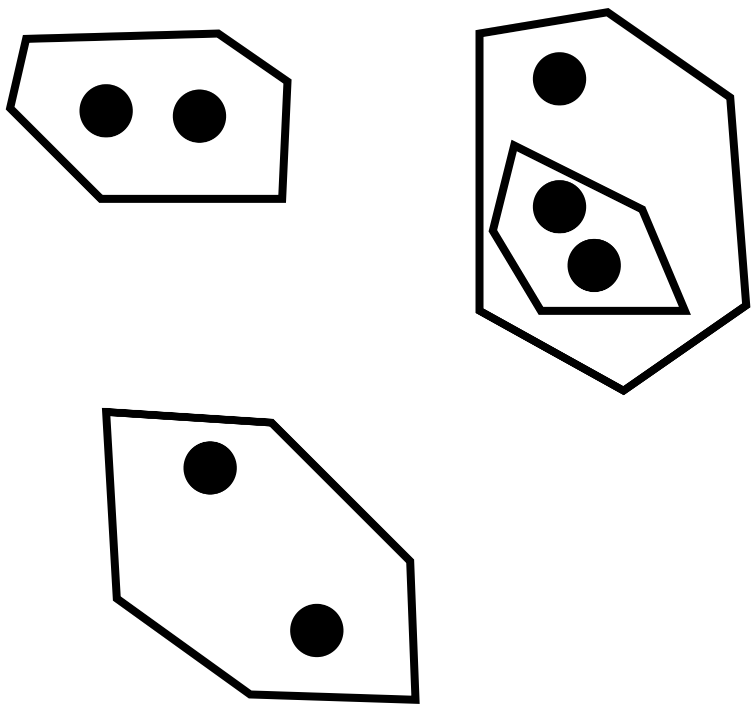
Bottom-up Clustering
single-link

- Step 2: compute the distance between all cluster pairs
- Step 3: merge/combine the nearest two clusters into one



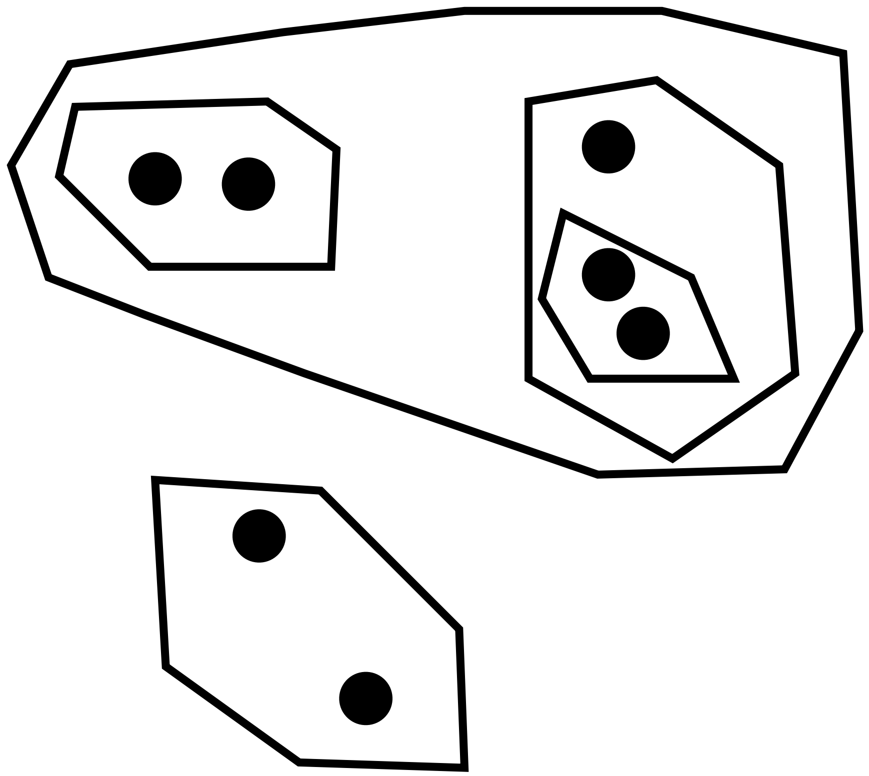
Bottom-up Clustering
single-link

- Step 2: compute the distance between all cluster pairs
- Step 3: merge/combine the nearest two clusters into one



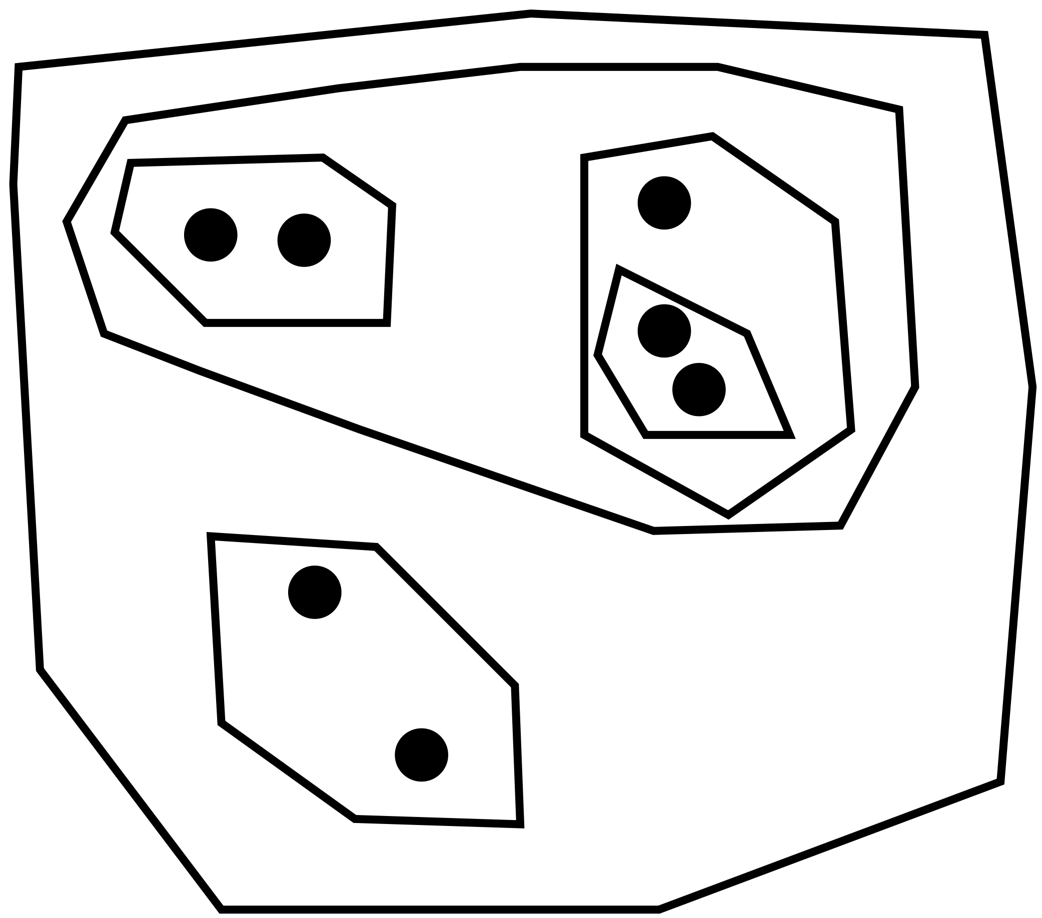
Bottom-up Clustering
single-link

- Step 2: compute the distance between all cluster pairs
- Step 3: merge/combine the nearest two clusters into one



Bottom-up Clustering
single-link

- Step 2: compute the distance between all cluster pairs
- Step 3: merge/combine the nearest two clusters into one



Bottom-up Clustering

- Setting K dynamically
- Instead of setting K, we could set a distance threshold T
- Stop merging/combining clusters when the distance between the two nearest clusters > T
- Using a distance threshold can help prevent "concept drift" (especially with single-link clustering)
    - text mining --> inls 613 --> unc --> basketball

Bottom-up Clustering

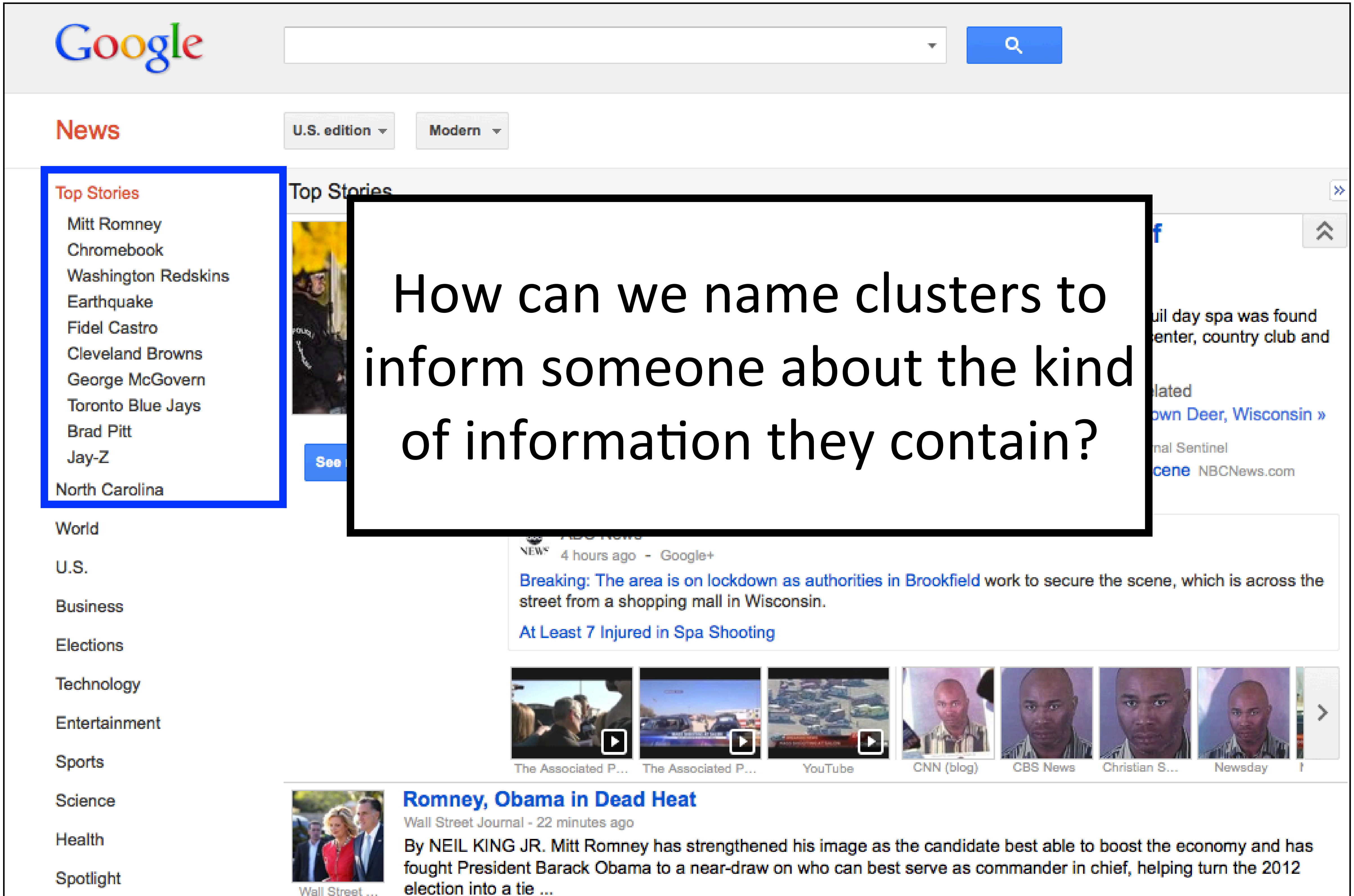
examples?

- Computing the distance between two clusters
- Single-Link: the distance between the two nearest documents
- Complete-Link: the distance between the two documents that are farthest apart
- Average-Link: the average distance between all document pairs (excluding those in the same cluster)
    - this is equivalent to using the distance between the two cluster centroids

Labeling Clusters

Clustering Applications

collection clustering



How can we name clusters to inform someone about the kind of information they contain?

Labeling Clusters

A simple solution

- Construct a vocabulary of terms and/or phrases (n-grams) that are frequent in the data
- Assign each cluster the term(s) or phrase(s) with the highest mutual information

Mutual Information

$$\mathrm{MI}(w, c) = \log\left(\frac{P(w, c)}{P(w)P(c)}\right)$$

- **P(w,c)**: the probability that a document contains word **w** and belongs to cluster **c**
- **P(w)**: the probability that word **w** occurs in a document from any cluster
- **P(c)**: the probability that a document belongs to cluster **c**

Mutual Information

$$\mathrm{MI}(w,c) = \log\left(\frac{P(w,c)}{P(w)P(c)}\right)$$

- If **P(w,c) = P(w) P(c)**, it means that the word **w** is independent of cluster **c**
- If **P(w,c) > P(w) P(c)**, it means that the word **w** is not independent of of cluster **c**

Mutual Information

- Every document falls under one of these quadrants

	belongs to cluster **c**	does not belong to cluster **c**
contains word **w**	a	b
does not contains word **w**	c	d

total # of instances N = a + b + c + d

P(w, c) = a / N

P(c) = (a + c) / N

P(w) = (a + b) / N

$$\mathrm{MI}(w,c) = \log\left(\frac{P(w,c)}{P(w)P(c)}\right)$$

Summary

- Clustering: grouping similar documents (or instances) into subsets
- Exploratory analysis: the goal is to discover common and uncommon properties of the data
- K-means and Agglomerative Bottom-up Clustering (there are many, many others)
- Labeling clusters